



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:01 AM EDT

PDB ID : 1MJG / pdb_00001mjg
Title : CRYSTAL STRUCTURE OF BIFUNCTIONAL CARBON MONOXIDE
DEHYDROGENASE / ACETYL-COA SYNTHASE(CODH/ACS)
FROM MOORELLA THERMOACETICA (F. CLOSTRIDIUM THER-
MOACETICUM)
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Deposited on : 2002-08-27
Resolution : 2.20 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

<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
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)	:	2.50

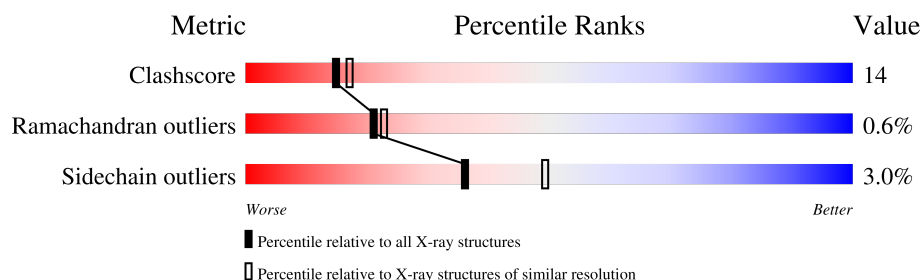
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	674	75% 22% .
1	B	674	75% 21% .
1	C	674	75% 22% .
1	D	674	75% 23% .
2	M	729	74% 23% .
2	N	729	73% 24% .
2	O	729	69% 27% .
2	P	729	71% 26% .

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	XCC	A	800	-	-	X	-
4	XCC	B	800	-	-	X	-
4	XCC	C	800	-	-	X	-
4	XCC	D	800	-	-	X	-
7	ACT	M	950	-	-	X	-
7	ACT	N	950	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44653 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 CARBON MONOXIDE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	B	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	C	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			
1	D	672	Total	C	N	O	S	0	0	0
			5087	3197	890	958	42			

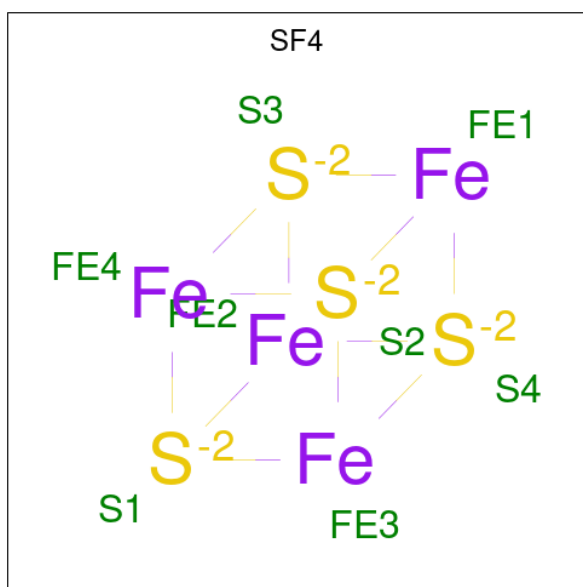
- Molecule 2 is a protein called Carbon monoxide dehydrogenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	N	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	O	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			
2	P	728	Total	C	N	O	S	0	0	0
			5735	3678	953	1069	35			

There are 4 discrepancies between the modelled and reference sequences:

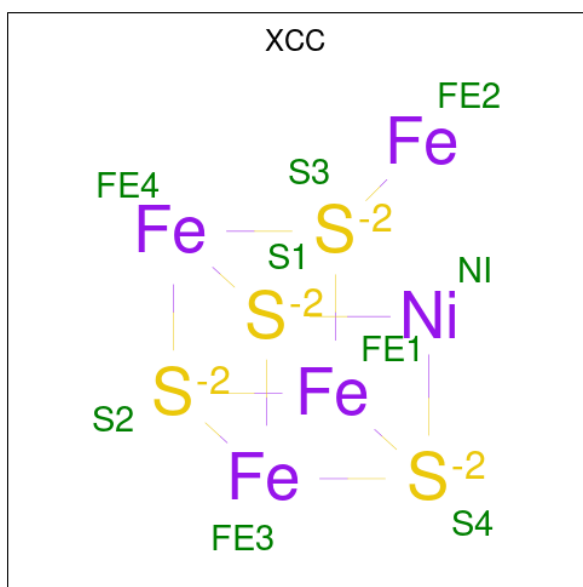
Chain	Residue	Modelled	Actual	Comment	Reference
M	685	SER	ARG	SEE REMARK 999	UNP P27988
N	685	SER	ARG	SEE REMARK 999	UNP P27988
O	685	SER	ARG	SEE REMARK 999	UNP P27988
P	685	SER	ARG	SEE REMARK 999	UNP P27988

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3	O	1	Total	Fe	S	0	0
			8	4	4		
3	P	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (CCD ID: XCC) (formula: Fe₄NiS₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	Cu	0	0
			1	1		
5	N	1	Total	Cu	0	0
			1	1		
5	O	1	Total	Cu	0	0
			1	1		
5	P	1	Total	Cu	0	0
			1	1		

- Molecule 6 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

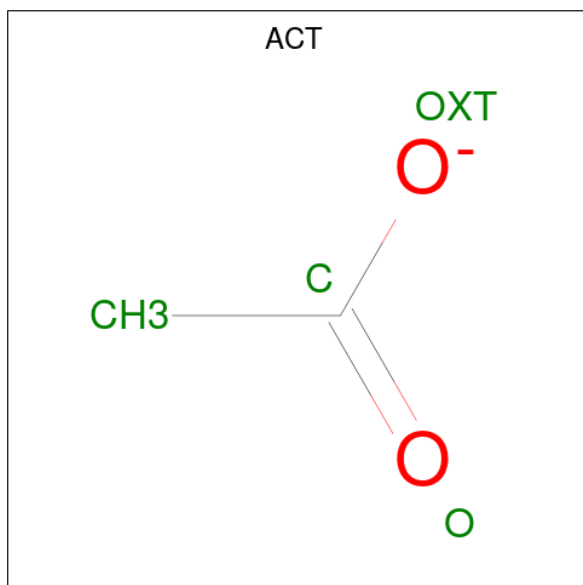
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total	Ni	0	0
			1	1		
6	O	1	Total	Ni	0	0
			1	1		
6	P	1	Total	Ni	0	0
			1	1		

- Molecule 7 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	M	1	Total	C	O	0	0
			3	2	1		
7	N	1	Total	C	O	0	0
			3	2	1		
7	O	1	Total	C	O	0	0
			3	2	1		
7	P	1	Total	C	O	0	0
			3	2	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	179	Total	O	0	0
			179	179		
8	B	217	Total	O	0	0
			217	217		

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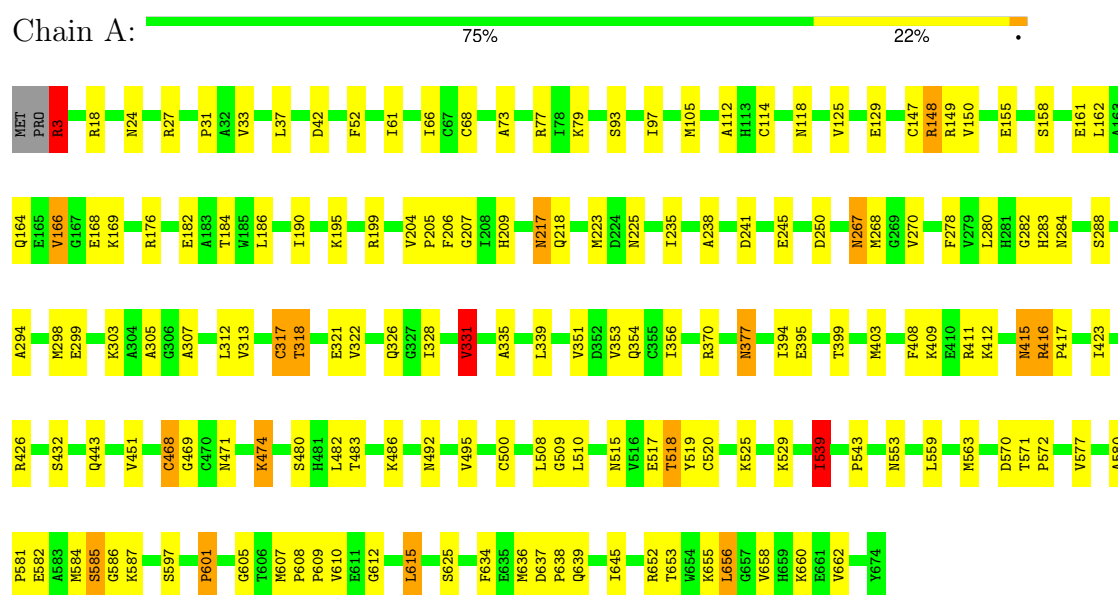
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	148	Total 148	O 148	0	0
8	D	131	Total 131	O 131	0	0
8	M	206	Total 206	O 206	0	0
8	N	221	Total 221	O 221	0	0
8	O	26	Total 26	O 26	0	0
8	P	101	Total 101	O 101	0	0

3 Residue-property plots [i](#)

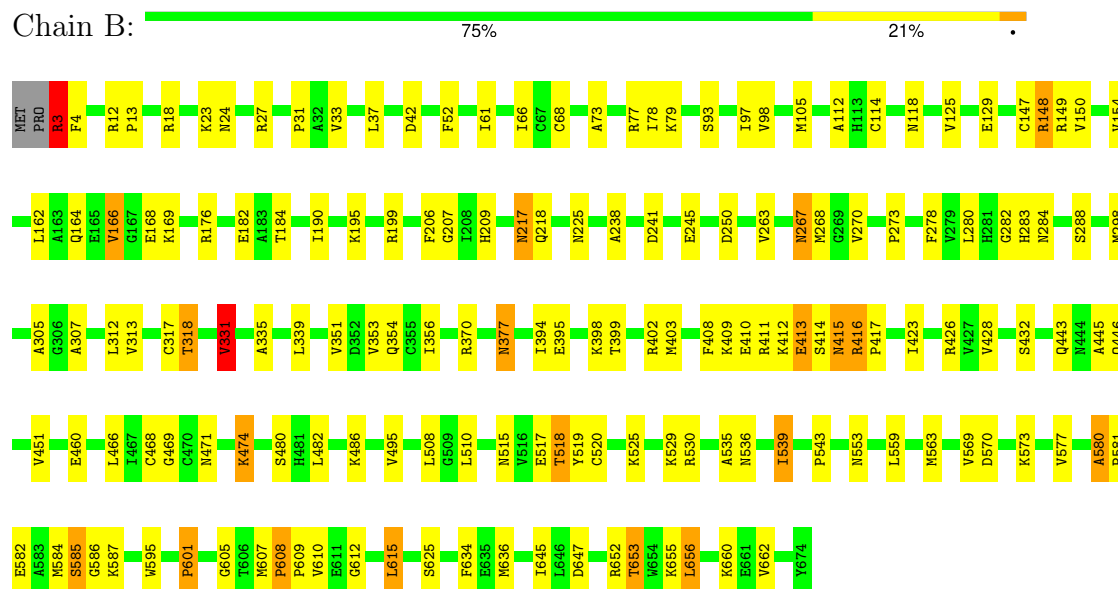
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

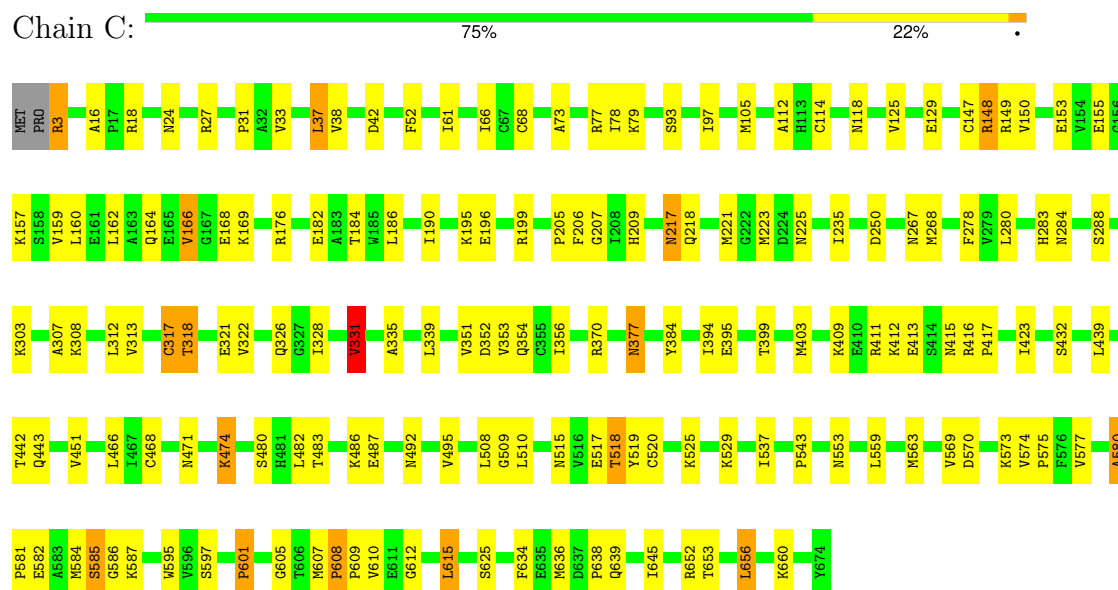
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



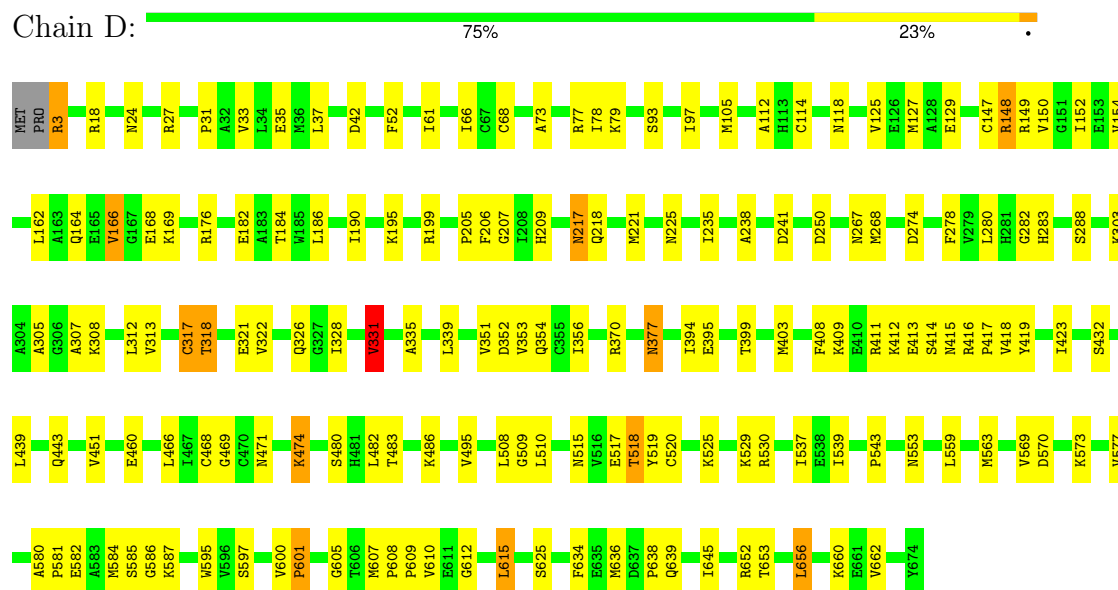
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



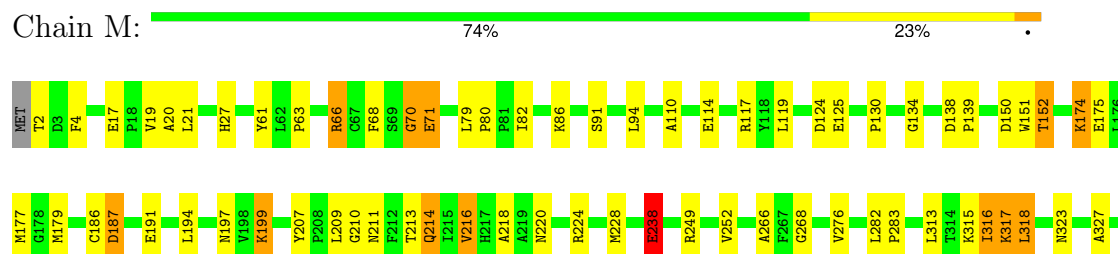
• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



• Molecule 1: CARBON MONOXIDE DEHYDROGENASE BETA SUBUNIT



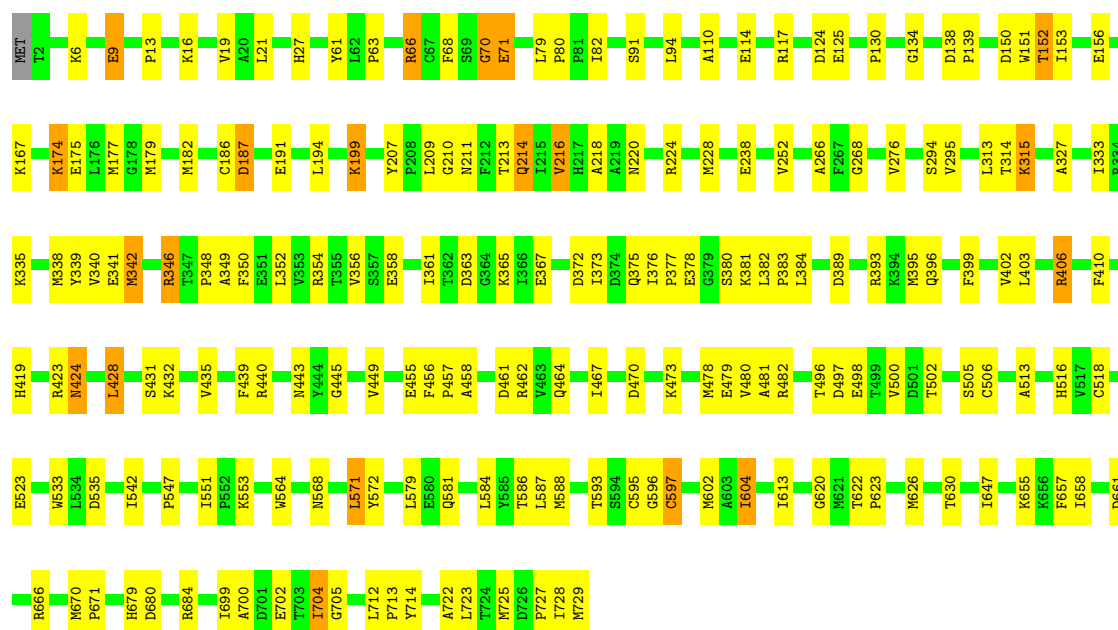
• Molecule 2: Carbon monoxide dehydrogenase alpha subunit





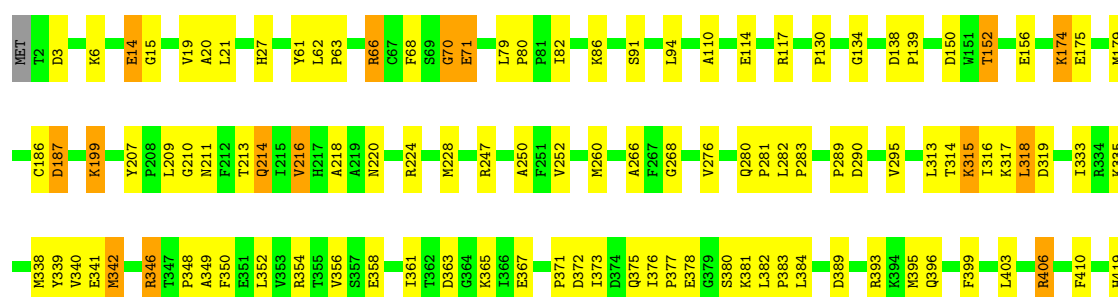
• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

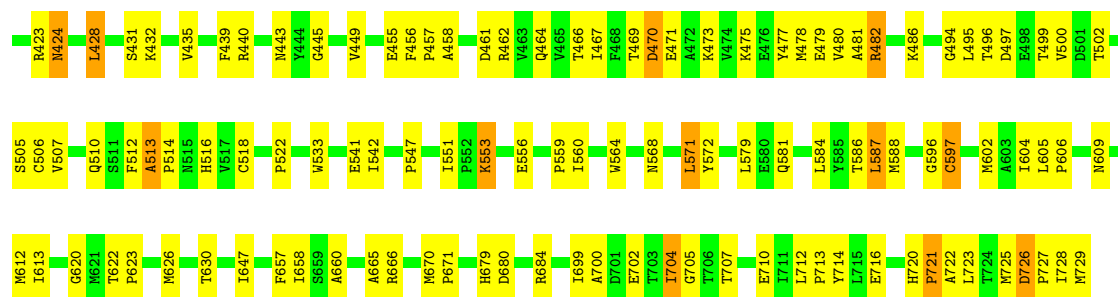
Chain N: 73% 24% .



• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

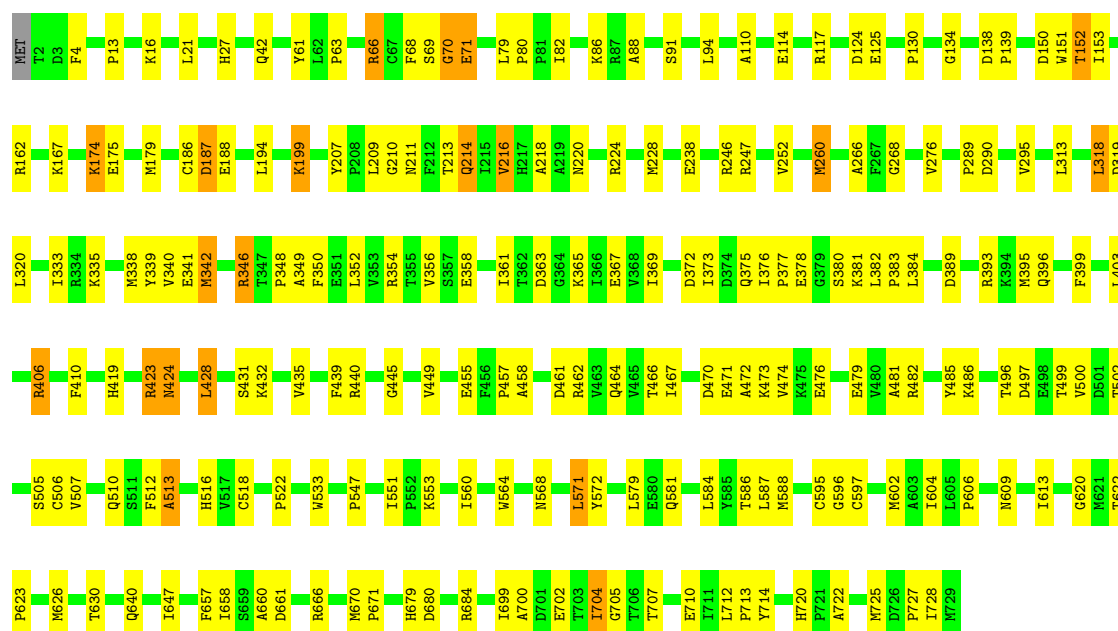
Chain O: 69% 27% .





• Molecule 2: Carbon monoxide dehydrogenase alpha subunit

Chain P: 71% 26%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.75Å 136.97Å 141.53Å 101.45° 109.05° 103.94°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	90.6 (20.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	44653	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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, ACT, XCC, CU1, NI

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	0.46	1/5179 (0.0%)	0.94	21/7017 (0.3%)
1	B	0.48	0/5179	0.95	19/7017 (0.3%)
1	C	0.43	0/5179	0.95	20/7017 (0.3%)
1	D	0.41	0/5179	0.93	14/7017 (0.2%)
2	M	0.42	0/5869	0.93	23/7948 (0.3%)
2	N	0.43	0/5869	0.93	21/7948 (0.3%)
2	O	0.35	0/5869	0.91	22/7948 (0.3%)
2	P	0.38	0/5869	0.91	23/7948 (0.3%)
All	All	0.42	1/44192 (0.0%)	0.93	163/59860 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	ARG	CZ-NH2	-5.25	1.26	1.33

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	CYS	N-CA-C	10.30	122.50	111.28
1	D	317	CYS	N-CA-C	10.12	122.31	111.28
1	A	317	CYS	N-CA-C	9.98	122.16	111.28
1	B	317	CYS	N-CA-C	9.86	122.03	111.28
2	M	152	THR	N-CA-C	-8.39	102.30	112.54
2	O	152	THR	N-CA-C	-8.38	102.15	112.38
2	P	152	THR	N-CA-C	-8.16	102.42	112.38
2	O	70	GLY	N-CA-C	8.09	126.08	115.40
2	N	152	THR	N-CA-C	-8.08	102.53	112.38
2	M	70	GLY	N-CA-C	7.87	125.79	115.40
2	N	513	ALA	CA-C-N	7.86	129.66	119.84
2	N	513	ALA	C-N-CA	7.86	129.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	70	GLY	N-CA-C	7.63	125.47	115.40
2	M	218	ALA	N-CA-C	-7.58	101.91	112.45
2	M	513	ALA	CA-C-N	7.57	129.30	119.84
2	M	513	ALA	C-N-CA	7.57	129.30	119.84
1	B	318	THR	N-CA-C	-7.48	103.14	111.82
2	N	70	GLY	N-CA-C	7.47	125.30	115.36
1	A	495	VAL	N-CA-C	7.39	118.92	108.36
2	O	218	ALA	N-CA-C	-7.34	102.24	112.45
1	A	318	THR	N-CA-C	-7.30	103.35	111.82
1	C	495	VAL	N-CA-C	7.27	118.75	108.36
2	P	218	ALA	N-CA-C	-7.24	102.39	112.45
1	C	318	THR	N-CA-C	-7.24	103.42	111.82
2	O	513	ALA	CA-C-N	7.22	128.87	119.84
2	O	513	ALA	C-N-CA	7.22	128.87	119.84
1	D	318	THR	N-CA-C	-7.22	103.41	111.71
1	D	495	VAL	N-CA-C	7.21	118.68	108.36
1	B	495	VAL	N-CA-C	7.14	118.57	108.36
2	P	513	ALA	CA-C-N	7.13	128.75	119.84
2	P	513	ALA	C-N-CA	7.13	128.75	119.84
1	B	268	MET	N-CA-C	7.04	120.76	111.75
2	N	346	ARG	N-CA-C	-6.88	105.17	113.97
1	A	268	MET	N-CA-C	6.85	121.25	112.34
2	N	218	ALA	N-CA-C	-6.84	102.94	112.45
2	P	346	ARG	N-CA-C	-6.81	105.25	113.97
2	O	346	ARG	N-CA-C	-6.80	105.27	113.97
1	D	268	MET	N-CA-C	6.73	121.09	112.34
2	M	346	ARG	N-CA-C	-6.72	105.37	113.97
1	A	474	LYS	N-CA-C	-6.71	104.36	112.54
1	C	268	MET	N-CA-C	6.69	121.03	112.34
1	D	474	LYS	N-CA-C	-6.61	104.48	112.54
1	B	601	PRO	N-CA-C	-6.48	101.02	110.80
2	O	207	TYR	N-CA-C	6.46	120.04	108.47
2	N	207	TYR	N-CA-C	6.43	119.98	108.47
1	C	474	LYS	N-CA-C	-6.40	104.58	112.38
2	M	238	GLU	CA-CB-CG	6.39	126.88	114.10
2	P	207	TYR	N-CA-C	6.38	119.90	108.47
1	B	474	LYS	N-CA-C	-6.37	104.39	111.71
2	N	728	ILE	N-CA-C	-6.34	102.94	111.44
1	B	553	ASN	N-CA-C	-6.34	104.64	112.38
1	D	553	ASN	N-CA-C	-6.34	104.80	112.54
2	P	268	GLY	N-CA-C	-6.28	104.73	112.77
2	O	268	GLY	N-CA-C	-6.27	104.74	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	586	GLY	N-CA-C	-6.24	105.01	113.37
2	P	134	GLY	N-CA-C	-6.21	100.78	111.47
2	N	268	GLY	N-CA-C	-6.20	105.06	113.37
2	M	207	TYR	N-CA-C	6.19	119.55	108.47
1	A	553	ASN	N-CA-C	-6.19	104.99	112.54
2	P	91	SER	N-CA-C	6.13	118.77	110.31
1	C	553	ASN	N-CA-C	-6.09	105.11	112.54
2	O	134	GLY	N-CA-C	-6.05	101.06	111.47
2	N	620	GLY	N-CA-C	6.04	118.98	112.33
2	M	91	SER	N-CA-C	6.04	118.64	110.31
1	A	601	PRO	N-CA-C	-6.03	101.70	110.80
2	O	91	SER	N-CA-C	6.02	118.62	110.31
1	B	154	VAL	N-CA-C	5.96	117.49	111.00
2	P	94	LEU	N-CA-C	5.95	118.35	109.25
1	C	432	SER	N-CA-C	-5.91	103.15	110.41
2	O	94	LEU	N-CA-C	5.90	118.35	108.96
1	D	601	PRO	N-CA-C	-5.90	101.89	110.80
2	N	91	SER	N-CA-C	5.89	118.43	110.31
2	N	134	GLY	N-CA-C	-5.87	101.37	111.47
1	C	601	PRO	N-CA-C	-5.87	101.94	110.80
2	N	498	GLU	N-CA-C	5.87	119.62	112.23
1	B	586	GLY	N-CA-C	-5.85	105.53	113.37
1	A	586	GLY	N-CA-C	-5.83	105.56	113.37
1	D	432	SER	N-CA-C	-5.82	103.26	110.41
1	B	432	SER	N-CA-C	-5.81	103.26	110.41
1	C	331	VAL	CB-CA-C	-5.79	104.46	112.04
2	M	134	GLY	N-CA-C	-5.78	101.53	111.47
2	M	268	GLY	N-CA-C	-5.78	105.38	112.77
1	C	586	GLY	N-CA-C	-5.74	105.67	113.37
2	M	620	GLY	N-CA-C	5.74	118.65	112.33
2	O	620	GLY	N-CA-C	5.72	118.62	112.33
1	A	331	VAL	CB-CA-C	-5.72	104.55	112.04
2	P	620	GLY	N-CA-C	5.71	118.61	112.33
2	N	68	PHE	N-CA-C	5.69	119.40	112.23
2	P	68	PHE	N-CA-C	5.65	119.35	112.23
2	O	68	PHE	N-CA-C	5.63	119.32	112.23
1	A	432	SER	N-CA-C	-5.62	103.50	110.41
2	N	130	PRO	N-CA-C	-5.62	105.08	110.47
2	P	79	LEU	N-CA-C	5.59	122.16	109.81
1	B	331	VAL	CB-CA-C	-5.57	104.74	112.04
2	M	94	LEU	N-CA-C	5.57	117.81	108.96
2	N	94	LEU	N-CA-C	5.57	117.81	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	238	GLU	CB-CG-CD	5.53	122.00	112.60
2	N	79	LEU	N-CA-C	5.52	122.00	109.81
2	M	80	PRO	N-CA-C	5.50	117.41	110.70
1	D	509	GLY	N-CA-C	5.49	122.90	115.32
2	M	130	PRO	N-CA-C	-5.49	105.20	110.47
1	C	585	SER	N-CA-C	5.41	117.51	110.43
1	B	570	ASP	N-CA-C	-5.39	103.27	110.55
2	N	80	PRO	N-CA-C	5.38	117.27	110.70
2	O	79	LEU	N-CA-C	5.38	121.71	109.81
2	P	80	PRO	N-CA-C	5.38	117.26	110.70
2	M	79	LEU	N-CA-C	5.37	121.68	109.81
2	O	80	PRO	N-CA-C	5.36	117.24	110.70
2	M	68	PHE	N-CA-C	5.34	118.95	112.23
2	P	246	ARG	N-CA-C	5.33	118.25	111.69
2	N	597	CYS	N-CA-CB	-5.32	102.79	110.56
1	C	570	ASP	N-CA-C	-5.32	103.37	110.55
1	D	585	SER	N-CA-C	5.32	117.39	110.43
1	B	580	ALA	CA-C-N	5.30	125.37	119.32
1	B	580	ALA	C-N-CA	5.30	125.37	119.32
1	B	3	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	A	539	ILE	N-CA-C	-5.26	105.25	110.62
1	D	570	ASP	N-CA-C	-5.26	103.45	110.55
2	M	423	ARG	CB-CA-C	-5.26	110.49	116.54
2	P	423	ARG	CB-CA-C	-5.24	110.52	116.54
2	O	130	PRO	N-CA-C	-5.23	105.45	110.47
1	B	585	SER	N-CA-C	5.22	117.27	110.43
1	C	284	ASN	N-CA-C	5.19	116.46	109.24
1	D	520	CYS	N-CA-C	5.19	118.40	110.20
1	A	570	ASP	N-CA-C	-5.19	103.55	110.55
1	A	509	GLY	N-CA-C	5.16	122.45	115.32
1	C	196	GLU	CA-CB-CG	5.16	124.42	114.10
2	O	423	ARG	CB-CA-C	-5.16	110.61	116.54
2	P	597	CYS	N-CA-CB	-5.16	103.03	110.56
1	A	155	GLU	N-CA-C	5.15	117.78	110.10
2	O	597	CYS	N-CA-CB	-5.15	103.04	110.56
1	A	585	SER	N-CA-C	5.14	117.17	110.43
1	C	580	ALA	CA-C-N	5.14	125.18	119.32
1	C	580	ALA	C-N-CA	5.14	125.18	119.32
2	M	595	CYS	CA-C-N	-5.12	111.37	121.41
2	M	595	CYS	C-N-CA	-5.12	111.37	121.41
1	A	520	CYS	N-CA-C	5.12	118.29	110.20
2	P	260	MET	N-CA-C	5.10	117.51	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	119	LEU	N-CA-C	-5.10	106.32	112.54
1	D	331	VAL	CB-CA-C	-5.08	105.38	112.04
2	N	423	ARG	CB-CA-C	-5.08	110.70	116.54
1	C	608	PRO	N-CA-C	-5.08	104.51	110.70
1	C	509	GLY	N-CA-C	5.06	122.31	115.32
2	P	720	HIS	CA-C-N	5.06	125.09	119.32
2	P	720	HIS	C-N-CA	5.06	125.09	119.32
1	A	353	VAL	N-CA-C	5.06	117.01	108.81
2	M	597	CYS	N-CA-CB	-5.06	103.17	110.56
1	B	608	PRO	N-CA-C	-5.06	104.53	110.70
2	P	42	GLN	N-CA-C	-5.06	105.84	111.36
2	P	130	PRO	N-CA-C	-5.05	105.62	110.47
1	A	492	ASN	N-CA-C	5.05	118.56	111.74
1	B	284	ASN	N-CA-C	5.05	116.26	109.24
1	C	520	CYS	N-CA-C	5.05	118.17	110.20
1	B	520	CYS	N-CA-C	5.04	118.17	110.20
1	C	492	ASN	N-CA-C	5.04	118.54	111.74
2	O	587	LEU	N-CA-C	-5.02	107.84	114.31
2	N	294	SER	N-CA-C	5.02	118.25	110.17
2	O	62	LEU	N-CA-C	-5.02	98.72	109.81
1	A	284	ASN	N-CA-C	5.01	116.21	109.24
1	A	468	CYS	CA-C-N	-5.01	115.33	122.64
1	A	468	CYS	C-N-CA	-5.01	115.33	122.64
2	O	62	LEU	CA-C-N	5.01	126.10	119.84
2	O	62	LEU	C-N-CA	5.01	126.10	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5087	0	5089	131	0
1	B	5087	0	5089	148	0
1	C	5087	0	5089	137	0
1	D	5087	0	5089	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	5735	0	5693	161	0
2	N	5735	0	5693	161	0
2	O	5735	0	5693	196	0
2	P	5735	0	5693	175	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	0	0
3	O	8	0	0	0	0
3	P	8	0	0	0	0
4	A	9	0	0	3	0
4	B	9	0	0	2	0
4	C	9	0	0	3	0
4	D	9	0	0	2	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	M	3	0	3	2	0
7	N	3	0	3	2	0
7	O	3	0	3	1	0
7	P	3	0	3	1	0
8	A	179	0	0	3	0
8	B	217	0	0	6	0
8	C	148	0	0	3	0
8	D	131	0	0	0	0
8	M	206	0	0	2	0
8	N	221	0	0	7	0
8	O	26	0	0	0	0
8	P	101	0	0	1	0
All	All	44653	0	43140	1193	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 14.

All (1193) 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:607:MET:HE3	1:B:608:PRO:HD2	1.33	1.11
1:C:607:MET:HE3	1:C:608:PRO:HD2	1.35	1.08
1:D:607:MET:HE3	1:D:608:PRO:HD2	1.35	1.07
2:O:335:LYS:H	2:O:335:LYS:HD2	1.21	1.06
1:A:607:MET:HE3	1:A:608:PRO:HD2	1.37	1.05
2:M:335:LYS:HD2	2:M:335:LYS:H	1.20	1.03
2:P:335:LYS:H	2:P:335:LYS:HD2	1.21	1.03
1:B:446:GLN:HE22	1:C:38:VAL:HG11	1.22	1.02
2:N:335:LYS:H	2:N:335:LYS:HD2	1.20	1.02
1:A:426:ARG:NH2	1:A:539:ILE:HG13	1.81	0.93
1:B:3:ARG:HH12	1:B:625:SER:CB	1.83	0.92
1:B:3:ARG:HG2	1:B:3:ARG:HH21	1.35	0.91
2:M:318:LEU:H	2:M:318:LEU:HD23	1.35	0.89
1:B:446:GLN:HE22	1:C:38:VAL:CG1	1.86	0.88
2:M:213:THR:O	2:M:216:VAL:HG23	1.73	0.88
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.55	0.88
2:P:318:LEU:HD23	2:P:318:LEU:H	1.38	0.88
1:A:3:ARG:NH2	1:A:625:SER:OG	2.06	0.88
1:B:263:VAL:HG22	1:B:539:ILE:HD12	1.57	0.87
1:B:428:VAL:HG22	1:B:539:ILE:HD11	1.55	0.86
2:N:71:GLU:HG3	2:N:82:ILE:HD11	1.56	0.86
2:N:213:THR:O	2:N:216:VAL:HG23	1.75	0.85
2:P:213:THR:O	2:P:216:VAL:HG23	1.76	0.85
1:D:274:ASP:HB2	1:D:308:LYS:HE2	1.54	0.85
2:O:602:MET:HE2	2:O:647:ILE:HD13	1.56	0.85
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.57	0.85
2:N:478:MET:O	2:N:482:ARG:HG2	1.77	0.84
1:B:446:GLN:NE2	1:C:38:VAL:HG11	1.92	0.84
1:B:313:VAL:HB	1:B:331:VAL:HG22	1.60	0.83
2:M:71:GLU:HG3	2:M:82:ILE:HD11	1.61	0.82
1:D:313:VAL:HB	1:D:331:VAL:HG22	1.59	0.82
1:B:412:LYS:HD3	1:B:416:ARG:HD3	1.61	0.82
2:O:213:THR:O	2:O:216:VAL:HG23	1.79	0.82
1:A:313:VAL:HB	1:A:331:VAL:HG22	1.61	0.82
1:B:482:LEU:HD12	1:B:486:LYS:HE3	1.62	0.81
1:A:3:ARG:HH22	1:A:625:SER:CB	1.93	0.80
1:B:93:SER:H	1:B:225:ASN:HD21	1.29	0.80
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.46	0.80
1:B:426:ARG:HH21	1:B:539:ILE:HG13	1.47	0.80
1:C:3:ARG:HH12	1:C:625:SER:CB	1.95	0.79
1:C:93:SER:H	1:C:225:ASN:HD21	1.30	0.79
1:C:313:VAL:HB	1:C:331:VAL:HG22	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:602:MET:HE2	2:N:647:ILE:HD13	1.64	0.79
1:B:263:VAL:CG2	1:B:539:ILE:HD12	2.13	0.78
2:P:71:GLU:HG3	2:P:82:ILE:HD11	1.64	0.77
2:P:700:ALA:HB1	2:P:704:ILE:HD11	1.67	0.77
2:P:604:ILE:HD12	2:P:604:ILE:O	1.84	0.77
1:A:482:LEU:HD12	1:A:486:LYS:HE3	1.67	0.77
1:A:426:ARG:HH22	1:A:539:ILE:HG13	1.50	0.77
1:D:93:SER:H	1:D:225:ASN:HD21	1.31	0.77
1:C:411:ARG:HG2	1:C:416:ARG:HD3	1.68	0.76
1:D:607:MET:HE3	1:D:608:PRO:CD	2.16	0.76
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.50	0.76
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.47	0.76
2:M:588:MET:HE1	2:M:604:ILE:CG2	2.15	0.76
2:P:335:LYS:H	2:P:335:LYS:CD	1.99	0.75
2:O:604:ILE:HD12	2:O:604:ILE:O	1.86	0.75
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.50	0.75
1:B:150:VAL:HG11	1:B:169:LYS:HG2	1.68	0.75
1:D:482:LEU:HD12	1:D:486:LYS:HE3	1.67	0.75
2:O:497:ASP:HA	2:O:500:VAL:HG12	1.67	0.75
1:B:607:MET:HE3	1:B:608:PRO:CD	2.14	0.75
2:O:352:LEU:HD22	2:O:481:ALA:HB2	1.69	0.75
2:N:335:LYS:H	2:N:335:LYS:CD	1.98	0.75
2:O:110:ALA:HB1	2:O:216:VAL:HG21	1.68	0.74
2:O:110:ALA:HB1	2:O:216:VAL:CG2	2.17	0.74
2:N:110:ALA:HB1	2:N:216:VAL:CG2	2.18	0.74
2:O:342:MET:HG3	2:O:384:LEU:HD22	1.69	0.74
1:A:607:MET:HE3	1:A:608:PRO:CD	2.17	0.74
2:M:604:ILE:O	2:M:604:ILE:HD12	1.87	0.74
2:P:588:MET:HE1	2:P:604:ILE:CG2	2.18	0.74
1:A:93:SER:H	1:A:225:ASN:HD21	1.34	0.74
1:B:148:ARG:HH11	1:B:148:ARG:HB3	1.52	0.74
1:C:482:LEU:HD12	1:C:486:LYS:HE3	1.69	0.74
1:A:148:ARG:HH11	1:A:148:ARG:HB3	1.52	0.74
1:A:283:HIS:N	1:A:318:THR:HG23	2.03	0.74
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.69	0.74
1:B:3:ARG:NH1	1:B:625:SER:OG	2.19	0.73
1:B:577:VAL:HG21	1:B:645:ILE:HG23	1.69	0.73
1:C:607:MET:HE3	1:C:608:PRO:CD	2.16	0.73
2:M:342:MET:HG3	2:M:384:LEU:HD22	1.69	0.73
2:P:110:ALA:HB1	2:P:216:VAL:CG2	2.18	0.73
1:C:150:VAL:HG11	1:C:169:LYS:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:71:GLU:HG3	2:N:82:ILE:CD1	2.17	0.73
1:A:150:VAL:HG11	1:A:169:LYS:HG2	1.70	0.73
1:D:615:LEU:HD23	2:P:27:HIS:HB3	1.69	0.73
2:O:335:LYS:H	2:O:335:LYS:CD	1.99	0.73
1:C:412:LYS:HZ2	1:C:416:ARG:HH21	1.37	0.73
1:D:150:VAL:HG11	1:D:169:LYS:HG2	1.69	0.73
1:D:411:ARG:NH1	1:D:416:ARG:HH21	1.86	0.73
2:N:377:PRO:HG2	2:N:380:SER:HB3	1.71	0.73
1:D:148:ARG:HB3	1:D:148:ARG:HH11	1.54	0.72
1:B:283:HIS:N	1:B:318:THR:HG23	2.04	0.72
2:M:71:GLU:HG3	2:M:82:ILE:CD1	2.19	0.72
2:O:588:MET:HE1	2:O:604:ILE:CG2	2.20	0.72
1:A:577:VAL:HG21	1:A:645:ILE:HG23	1.72	0.72
1:C:148:ARG:HH11	1:C:148:ARG:HB3	1.55	0.72
2:P:377:PRO:HG2	2:P:380:SER:HB3	1.72	0.72
1:C:577:VAL:HG21	1:C:645:ILE:HG23	1.72	0.71
2:P:71:GLU:HG3	2:P:82:ILE:CD1	2.20	0.71
1:B:469:GLY:HA3	8:B:889:HOH:O	1.90	0.70
1:D:3:ARG:HH22	1:D:625:SER:CB	2.03	0.70
1:C:283:HIS:N	1:C:318:THR:HG23	2.05	0.70
2:N:342:MET:HG3	2:N:384:LEU:HD22	1.72	0.70
1:C:412:LYS:NZ	1:C:416:ARG:HH21	1.88	0.70
1:D:283:HIS:N	1:D:318:THR:HG23	2.07	0.70
2:N:63:PRO:HB2	2:N:220:ASN:HB2	1.73	0.70
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.73	0.70
2:O:377:PRO:HG2	2:O:380:SER:HB3	1.72	0.70
2:O:342:MET:HG2	2:O:428:LEU:HB2	1.72	0.70
1:B:23:LYS:HD3	8:B:851:HOH:O	1.92	0.70
2:M:110:ALA:HB1	2:M:216:VAL:CG2	2.22	0.70
2:N:586:THR:HG22	2:N:588:MET:H	1.57	0.70
1:B:3:ARG:NH1	1:B:625:SER:CB	2.55	0.70
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.72	0.70
1:D:577:VAL:HG21	1:D:645:ILE:HG23	1.73	0.70
2:M:335:LYS:H	2:M:335:LYS:CD	1.99	0.69
2:O:110:ALA:CB	2:O:216:VAL:HG21	2.22	0.69
2:O:365:LYS:HB3	2:O:464:GLN:HG3	1.74	0.69
2:P:365:LYS:HB3	2:P:464:GLN:HG3	1.74	0.69
2:O:338:MET:SD	2:O:341:GLU:HB2	2.33	0.69
2:P:318:LEU:H	2:P:318:LEU:CD2	2.03	0.69
1:B:182:GLU:OE2	1:B:199:ARG:HD3	1.93	0.69
1:B:426:ARG:NH2	1:B:539:ILE:HG13	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:350:PHE:HB3	2:O:478:MET:HE1	1.74	0.69
1:B:263:VAL:HG22	1:B:539:ILE:CD1	2.23	0.69
2:N:335:LYS:HD2	2:N:335:LYS:N	2.02	0.69
2:M:377:PRO:HG2	2:M:380:SER:HB3	1.73	0.69
2:M:587:LEU:HB3	2:M:588:MET:HE2	1.75	0.68
2:N:365:LYS:HB3	2:N:464:GLN:HG3	1.75	0.68
2:P:342:MET:HG2	2:P:428:LEU:HB2	1.74	0.68
1:B:411:ARG:O	1:B:416:ARG:HB3	1.93	0.68
2:M:586:THR:HG22	2:M:588:MET:H	1.58	0.68
2:P:369:ILE:HG21	2:P:473:LYS:HD2	1.75	0.68
1:B:415:ASN:O	1:B:417:PRO:HD3	1.94	0.68
1:B:428:VAL:CG2	1:B:539:ILE:HD11	2.24	0.68
2:P:335:LYS:HD2	2:P:335:LYS:N	2.04	0.68
2:N:342:MET:HG2	2:N:428:LEU:HB2	1.74	0.68
2:N:500:VAL:HG21	2:N:533:TRP:CZ2	2.28	0.68
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.57	0.68
1:C:615:LEU:HD23	2:O:27:HIS:HB3	1.74	0.68
2:M:342:MET:HG2	2:M:428:LEU:HB2	1.76	0.68
1:D:482:LEU:HD21	1:D:508:LEU:HD12	1.75	0.67
1:B:3:ARG:HH21	1:B:3:ARG:CG	2.07	0.67
2:P:63:PRO:HB2	2:P:220:ASN:HB2	1.75	0.67
1:D:411:ARG:HH12	1:D:416:ARG:HH21	1.42	0.67
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.25	0.67
2:O:439:PHE:O	2:O:440:ARG:HD2	1.95	0.67
1:B:416:ARG:O	1:B:416:ARG:HG3	1.93	0.67
2:P:338:MET:SD	2:P:341:GLU:HB2	2.34	0.67
1:D:182:GLU:OE2	1:D:199:ARG:HD3	1.95	0.67
2:O:500:VAL:HG21	2:O:533:TRP:CZ2	2.30	0.67
2:P:439:PHE:O	2:P:440:ARG:HD2	1.95	0.67
2:M:721:PRO:O	2:M:725:MET:HG3	1.94	0.67
2:N:424:ASN:H	2:N:424:ASN:HD22	1.42	0.67
2:N:587:LEU:HB3	2:N:588:MET:HE2	1.77	0.67
2:N:727:PRO:HG2	2:N:729:MET:HE2	1.78	0.66
1:C:182:GLU:OE2	1:C:199:ARG:HD3	1.95	0.66
2:P:211:ASN:H	2:P:214:GLN:NE2	1.92	0.66
2:O:348:PRO:HG2	2:O:383:PRO:HB3	1.77	0.66
2:O:700:ALA:HB1	2:O:704:ILE:HD11	1.77	0.66
2:P:586:THR:HG22	2:P:588:MET:H	1.59	0.66
2:M:365:LYS:HB3	2:M:464:GLN:HG3	1.77	0.66
2:M:500:VAL:HG21	2:M:533:TRP:CZ2	2.30	0.66
2:P:110:ALA:HB1	2:P:216:VAL:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:439:PHE:O	2:M:440:ARG:HD2	1.96	0.66
2:O:587:LEU:HB3	2:O:588:MET:HE2	1.77	0.66
2:O:335:LYS:HD2	2:O:335:LYS:N	2.04	0.66
2:P:587:LEU:HB3	2:P:588:MET:HE2	1.77	0.66
2:M:424:ASN:HD22	2:M:424:ASN:H	1.43	0.66
2:P:500:VAL:HG21	2:P:533:TRP:CZ2	2.30	0.66
1:B:662:VAL:HG21	2:N:194:LEU:HD13	1.77	0.65
2:M:588:MET:HE1	2:M:604:ILE:HG21	1.78	0.65
2:M:335:LYS:HD2	2:M:335:LYS:N	2.02	0.65
2:N:110:ALA:HB1	2:N:216:VAL:HG21	1.76	0.65
1:B:482:LEU:HD21	1:B:508:LEU:HD12	1.79	0.65
2:M:252:VAL:HB	2:M:276:VAL:HG22	1.79	0.65
2:P:358:GLU:HG3	2:P:462:ARG:NH1	2.12	0.65
2:N:13:PRO:HB2	2:N:16:LYS:HG3	1.79	0.65
2:N:315:LYS:HZ2	2:N:315:LYS:HB3	1.61	0.65
2:P:383:PRO:HG2	2:P:471:GLU:HB2	1.78	0.65
1:C:377:ASN:H	1:C:377:ASN:HD22	1.45	0.65
2:O:424:ASN:HD22	2:O:424:ASN:H	1.44	0.65
2:M:211:ASN:H	2:M:214:GLN:NE2	1.95	0.65
2:O:358:GLU:HG3	2:O:462:ARG:NH1	2.12	0.65
4:C:800:XCC:S3	4:C:800:XCC:FE2	1.89	0.64
2:N:439:PHE:O	2:N:440:ARG:HD2	1.96	0.64
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.62	0.64
1:C:377:ASN:H	1:C:377:ASN:ND2	1.96	0.64
2:P:497:ASP:HA	2:P:500:VAL:HG12	1.78	0.64
2:M:63:PRO:HB2	2:M:220:ASN:HB2	1.80	0.64
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.62	0.64
2:O:477:TYR:HA	2:O:480:VAL:HG23	1.79	0.64
2:O:586:THR:HG22	2:O:588:MET:H	1.60	0.64
2:M:354:ARG:HH21	2:M:480:VAL:HG11	1.62	0.64
1:C:482:LEU:HD21	1:C:508:LEU:HD12	1.80	0.64
1:D:559:LEU:HG	1:D:563:MET:CE	2.28	0.64
2:M:151:TRP:CH2	2:M:249:ARG:NH1	2.65	0.64
2:N:348:PRO:HG2	2:N:383:PRO:HB3	1.78	0.64
2:O:252:VAL:HB	2:O:276:VAL:HG22	1.78	0.64
2:P:110:ALA:CB	2:P:216:VAL:HG21	2.28	0.64
1:A:182:GLU:OE2	1:A:199:ARG:HD3	1.98	0.64
2:P:348:PRO:HG2	2:P:383:PRO:HB3	1.80	0.64
2:P:424:ASN:H	2:P:424:ASN:HD22	1.44	0.64
1:A:162:LEU:O	1:A:166:VAL:HG22	1.98	0.63
1:A:164:GLN:O	1:A:168:GLU:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HG	1:A:563:MET:CE	2.28	0.63
1:C:195:LYS:O	1:C:199:ARG:HG3	1.98	0.63
2:N:354:ARG:HH21	2:N:480:VAL:HG11	1.61	0.63
1:C:77:ARG:NH1	1:C:79:LYS:HE2	2.13	0.63
2:M:177:MET:HE2	2:M:327:ALA:HB1	1.80	0.63
2:M:110:ALA:HB1	2:M:216:VAL:HG21	1.81	0.63
2:M:354:ARG:NH2	2:M:480:VAL:HG11	2.14	0.63
1:D:77:ARG:NH1	1:D:79:LYS:HE2	2.13	0.63
2:N:358:GLU:HG3	2:N:462:ARG:NH1	2.14	0.63
2:O:497:ASP:OD1	2:O:522:PRO:HD2	1.99	0.63
1:B:559:LEU:HG	1:B:563:MET:CE	2.29	0.63
2:M:373:ILE:HD11	2:M:435:VAL:HG22	1.80	0.63
2:N:588:MET:HE1	2:N:604:ILE:CG2	2.29	0.62
2:O:470:ASP:HB3	2:O:473:LYS:HB2	1.79	0.62
1:A:469:GLY:HA3	8:A:921:HOH:O	1.99	0.62
2:N:339:TYR:CD2	2:N:435:VAL:HG21	2.34	0.62
2:O:373:ILE:HD11	2:O:435:VAL:HG22	1.80	0.62
1:A:3:ARG:HG2	1:A:3:ARG:HH11	1.64	0.62
2:N:211:ASN:H	2:N:214:GLN:NE2	1.98	0.62
2:O:475:LYS:HA	2:O:478:MET:HB2	1.80	0.62
1:B:3:ARG:HD2	8:N:1339:HOH:O	1.99	0.62
2:N:110:ALA:CB	2:N:216:VAL:HG21	2.29	0.62
2:P:318:LEU:HG	2:P:320:LEU:HG	1.80	0.62
1:A:482:LEU:HD21	1:A:508:LEU:HD12	1.82	0.62
2:P:467:ILE:N	2:P:467:ILE:HD12	2.15	0.62
1:D:164:GLN:O	1:D:168:GLU:HG3	1.99	0.62
2:N:167:LYS:HG2	8:N:1300:HOH:O	1.98	0.62
2:O:497:ASP:CA	2:O:500:VAL:HG12	2.30	0.62
2:N:352:LEU:HD22	2:N:481:ALA:HB2	1.80	0.62
2:O:313:LEU:O	2:O:313:LEU:HD12	2.00	0.62
1:B:114:CYS:SG	1:B:209:HIS:CE1	2.93	0.62
1:D:162:LEU:O	1:D:166:VAL:HG22	2.00	0.62
2:P:588:MET:HE1	2:P:604:ILE:HG21	1.81	0.62
2:O:399:PHE:HZ	2:O:541:GLU:HG3	1.65	0.61
1:B:428:VAL:HG22	1:B:539:ILE:CD1	2.27	0.61
2:P:373:ILE:HD11	2:P:435:VAL:HG22	1.82	0.61
1:A:468:CYS:O	1:A:580:ALA:HA	2.00	0.61
1:D:195:LYS:O	1:D:199:ARG:HG3	2.00	0.61
2:O:482:ARG:HA	2:O:482:ARG:NH1	2.15	0.61
1:C:164:GLN:O	1:C:168:GLU:HG3	1.99	0.61
2:N:349:ALA:HA	2:N:384:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.65	0.61
2:N:150:ASP:OD2	2:N:152:THR:HG23	2.01	0.61
2:N:373:ILE:HD11	2:N:435:VAL:HG22	1.82	0.61
1:B:164:GLN:O	1:B:168:GLU:HG3	2.01	0.61
2:M:348:PRO:HG2	2:M:383:PRO:HB3	1.81	0.61
1:B:412:LYS:HZ3	1:B:416:ARG:CZ	2.13	0.61
2:M:339:TYR:HD2	2:M:340:VAL:HG23	1.64	0.61
2:O:339:TYR:HD2	2:O:340:VAL:HG23	1.65	0.61
2:P:318:LEU:HD23	2:P:318:LEU:N	2.12	0.61
2:P:722:ALA:HA	2:P:725:MET:CE	2.31	0.61
2:O:349:ALA:HA	2:O:384:LEU:O	2.00	0.60
2:O:348:PRO:HB3	2:O:475:LYS:NZ	2.16	0.60
2:P:313:LEU:HD12	2:P:313:LEU:O	2.01	0.60
1:B:468:CYS:O	1:B:580:ALA:HA	2.02	0.60
2:P:339:TYR:HD2	2:P:340:VAL:HG23	1.65	0.60
2:O:588:MET:HE1	2:O:604:ILE:HG21	1.83	0.60
1:A:662:VAL:HG21	2:M:194:LEU:HD13	1.83	0.60
2:O:110:ALA:CB	2:O:216:VAL:CG2	2.79	0.60
2:M:338:MET:SD	2:M:341:GLU:HB2	2.41	0.60
2:P:252:VAL:HB	2:P:276:VAL:HG22	1.82	0.60
1:B:77:ARG:NH1	1:B:79:LYS:HE2	2.16	0.60
1:A:114:CYS:SG	1:A:209:HIS:CE1	2.95	0.60
1:B:607:MET:HE1	1:B:634:PHE:CD1	2.36	0.60
2:M:349:ALA:HA	2:M:384:LEU:O	2.01	0.60
1:B:298:MET:HE1	1:B:402:ARG:HG2	1.84	0.59
2:O:494:GLY:O	2:O:499:THR:HG21	2.02	0.59
2:O:211:ASN:H	2:O:214:GLN:NE2	2.00	0.59
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.18	0.59
1:A:148:ARG:HB3	1:A:148:ARG:NH1	2.17	0.59
2:N:500:VAL:HG22	2:N:502:THR:H	1.68	0.59
2:O:339:TYR:CD2	2:O:435:VAL:HG21	2.38	0.59
2:O:597:CYS:HB3	7:O:950:ACT:H1	1.85	0.59
2:M:313:LEU:O	2:M:313:LEU:HD12	2.02	0.59
2:O:406:ARG:HB3	2:O:406:ARG:NH1	2.17	0.59
2:O:467:ILE:HD12	2:O:467:ILE:N	2.17	0.59
2:P:110:ALA:CB	2:P:216:VAL:CG2	2.81	0.59
1:C:411:ARG:HG2	1:C:416:ARG:CD	2.32	0.59
2:M:339:TYR:CD2	2:M:435:VAL:HG21	2.38	0.59
1:C:3:ARG:NH1	1:C:625:SER:CB	2.65	0.59
1:D:615:LEU:HD23	2:P:27:HIS:CB	2.32	0.59
1:B:195:LYS:O	1:B:199:ARG:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:MET:HE1	1:D:634:PHE:CD1	2.37	0.59
1:A:195:LYS:O	1:A:199:ARG:HG3	2.02	0.59
1:A:607:MET:HE1	1:A:634:PHE:CD1	2.38	0.59
1:D:468:CYS:O	1:D:580:ALA:HA	2.02	0.59
2:O:187:ASP:HA	2:O:211:ASN:ND2	2.17	0.59
2:O:604:ILE:HD12	2:O:604:ILE:C	2.28	0.59
1:C:162:LEU:O	1:C:166:VAL:HG22	2.02	0.59
2:P:349:ALA:HA	2:P:384:LEU:O	2.01	0.59
1:A:607:MET:HE2	1:A:610:VAL:HG22	1.83	0.58
1:C:468:CYS:O	1:C:580:ALA:HA	2.02	0.58
2:P:516:HIS:HE1	2:P:518:CYS:SG	2.26	0.58
2:N:497:ASP:N	2:N:523:GLU:OE2	2.25	0.58
1:C:559:LEU:HG	1:C:563:MET:CE	2.32	0.58
1:C:335:ALA:H	1:C:471:ASN:HD22	1.50	0.58
2:N:339:TYR:HD2	2:N:340:VAL:HG23	1.67	0.58
2:N:338:MET:SD	2:N:341:GLU:HB2	2.44	0.58
2:N:470:ASP:OD2	2:N:473:LYS:HG2	2.03	0.58
1:A:77:ARG:NH1	1:A:79:LYS:HE2	2.19	0.58
1:D:482:LEU:CD2	1:D:508:LEU:HD12	2.33	0.58
2:M:339:TYR:CD2	2:M:340:VAL:HG23	2.39	0.58
2:P:187:ASP:HA	2:P:211:ASN:ND2	2.17	0.58
1:A:335:ALA:H	1:A:471:ASN:HD22	1.51	0.58
1:B:118:ASN:C	1:B:118:ASN:HD22	2.12	0.58
2:M:500:VAL:HG22	2:M:502:THR:H	1.67	0.58
2:N:313:LEU:HD12	2:N:313:LEU:O	2.03	0.58
2:O:477:TYR:HA	2:O:480:VAL:CG2	2.33	0.58
2:N:110:ALA:CB	2:N:216:VAL:CG2	2.82	0.58
2:O:175:GLU:HG2	2:O:179:MET:HE2	1.85	0.58
2:O:339:TYR:CD2	2:O:340:VAL:HG23	2.38	0.58
1:C:615:LEU:CD2	2:O:27:HIS:HB3	2.33	0.57
1:D:114:CYS:SG	1:D:209:HIS:CE1	2.97	0.57
2:P:339:TYR:CD2	2:P:340:VAL:HG23	2.39	0.57
2:P:395:MET:HE3	2:P:396:GLN:O	2.04	0.57
2:P:604:ILE:HD12	2:P:604:ILE:C	2.28	0.57
1:B:148:ARG:HB3	1:B:148:ARG:NH1	2.17	0.57
1:C:515:ASN:HA	1:C:518:THR:HG23	1.86	0.57
2:N:372:ASP:H	2:N:375:GLN:NE2	2.01	0.57
1:C:615:LEU:HD23	2:O:27:HIS:CB	2.34	0.57
1:A:3:ARG:NH2	1:A:625:SER:CB	2.65	0.57
1:A:118:ASN:C	1:A:118:ASN:HD22	2.13	0.57
1:B:335:ALA:H	1:B:471:ASN:HD22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:LYS:HE3	4:C:800:XCC:S4	2.44	0.57
2:M:700:ALA:HB1	2:M:704:ILE:HD11	1.87	0.57
1:B:162:LEU:O	1:B:166:VAL:HG22	2.05	0.57
1:B:482:LEU:CD2	1:B:508:LEU:HD12	2.35	0.57
2:M:318:LEU:H	2:M:318:LEU:CD2	2.14	0.57
1:A:377:ASN:H	1:A:377:ASN:ND2	2.02	0.57
1:D:416:ARG:NH2	1:D:418:VAL:HG21	2.20	0.57
1:A:33:VAL:HG13	1:A:339:LEU:HD12	1.87	0.57
1:D:615:LEU:CD2	2:P:27:HIS:HB3	2.35	0.57
2:M:110:ALA:CB	2:M:216:VAL:HG21	2.35	0.57
2:M:151:TRP:CZ3	2:M:249:ARG:NH1	2.69	0.57
2:O:728:ILE:HG12	2:O:728:ILE:O	2.05	0.57
2:P:352:LEU:HD22	2:P:481:ALA:HB2	1.86	0.57
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.85	0.56
2:M:317:LYS:HB2	2:M:317:LYS:NZ	2.20	0.56
2:P:339:TYR:HB2	2:P:432:LYS:HA	1.87	0.56
1:A:607:MET:HE2	1:A:610:VAL:CG2	2.35	0.56
1:B:585:SER:OG	4:B:800:XCC:S4	2.62	0.56
1:C:33:VAL:HG13	1:C:339:LEU:HD12	1.86	0.56
2:M:467:ILE:HD12	2:M:467:ILE:N	2.20	0.56
2:M:604:ILE:HD12	2:M:604:ILE:C	2.30	0.56
2:O:348:PRO:HG3	2:O:475:LYS:HE2	1.87	0.56
1:D:148:ARG:HB3	1:D:148:ARG:NH1	2.20	0.56
2:N:177:MET:HE2	2:N:327:ALA:HB1	1.87	0.56
2:N:700:ALA:HB1	2:N:704:ILE:HD11	1.88	0.56
2:O:506:CYS:HA	2:O:547:PRO:O	2.05	0.56
2:N:595:CYS:HB2	7:N:950:ACT:H1	1.86	0.56
2:P:333:ILE:HD12	2:P:431:SER:HB3	1.87	0.56
2:P:339:TYR:CD2	2:P:435:VAL:HG21	2.41	0.56
1:B:351:VAL:HG22	1:B:356:ILE:CD1	2.34	0.56
2:P:496:THR:OG1	2:P:499:THR:HG23	2.06	0.56
1:A:426:ARG:HH21	1:A:539:ILE:HG13	1.67	0.56
1:C:114:CYS:SG	1:C:209:HIS:CE1	2.99	0.56
1:C:482:LEU:CD2	1:C:508:LEU:HD12	2.36	0.56
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.21	0.56
2:M:187:ASP:HA	2:M:211:ASN:ND2	2.19	0.56
2:O:395:MET:HE3	2:O:396:GLN:O	2.06	0.56
2:M:339:TYR:HB2	2:M:432:LYS:HA	1.88	0.56
2:N:467:ILE:N	2:N:467:ILE:HD12	2.21	0.56
2:O:516:HIS:HE1	2:O:518:CYS:SG	2.28	0.56
1:A:307:ALA:HB2	1:A:408:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:333:ILE:HD12	2:M:431:SER:HB3	1.88	0.55
2:O:571:LEU:HD22	2:O:579:LEU:HB2	1.88	0.55
2:P:700:ALA:CB	2:P:704:ILE:HD11	2.35	0.55
1:B:33:VAL:HG13	1:B:339:LEU:HD12	1.89	0.55
2:M:372:ASP:H	2:M:375:GLN:NE2	2.05	0.55
2:M:516:HIS:HE1	2:M:518:CYS:SG	2.29	0.55
2:O:61:TYR:O	2:O:63:PRO:HD3	2.06	0.55
2:M:174:LYS:NZ	2:M:174:LYS:HB3	2.21	0.55
2:N:406:ARG:HB3	2:N:406:ARG:NH1	2.22	0.55
2:P:406:ARG:NH1	2:P:406:ARG:HB3	2.20	0.55
1:B:147:CYS:SG	1:B:166:VAL:HG13	2.46	0.55
2:N:571:LEU:HD22	2:N:579:LEU:HB2	1.88	0.55
2:O:333:ILE:HD12	2:O:431:SER:HB3	1.87	0.55
2:O:393:ARG:HG2	2:O:461:ASP:OD2	2.06	0.55
2:O:495:LEU:HD21	2:O:533:TRP:CZ3	2.41	0.55
1:D:515:ASN:HA	1:D:518:THR:HG23	1.89	0.55
2:O:224:ARG:O	2:O:228:MET:HG3	2.07	0.55
2:P:342:MET:HB3	2:P:382:LEU:O	2.07	0.55
1:A:66:ILE:HG23	1:A:612:GLY:HA3	1.88	0.55
1:C:153:GLU:OE2	1:C:155:GLU:HG3	2.07	0.55
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.89	0.55
2:N:339:TYR:HB2	2:N:432:LYS:HA	1.88	0.55
2:N:342:MET:HB3	2:N:382:LEU:O	2.07	0.55
1:A:33:VAL:HG13	1:A:339:LEU:CD1	2.37	0.55
1:A:415:ASN:O	1:A:417:PRO:HD3	2.06	0.55
2:N:252:VAL:HB	2:N:276:VAL:HG22	1.89	0.55
2:N:395:MET:HE3	2:N:396:GLN:O	2.07	0.55
1:D:335:ALA:H	1:D:471:ASN:HD22	1.53	0.54
2:M:342:MET:HB3	2:M:382:LEU:O	2.07	0.54
2:M:406:ARG:HB3	2:M:406:ARG:NH1	2.22	0.54
2:N:704:ILE:HD13	2:N:714:TYR:CG	2.42	0.54
2:O:496:THR:O	2:O:500:VAL:N	2.40	0.54
1:C:118:ASN:C	1:C:118:ASN:HD22	2.15	0.54
2:N:373:ILE:CD1	2:N:435:VAL:HG22	2.37	0.54
2:O:314:THR:O	2:O:316:ILE:N	2.40	0.54
1:A:77:ARG:HD3	8:A:865:HOH:O	2.07	0.54
2:N:393:ARG:HG2	2:N:461:ASP:OD2	2.07	0.54
2:P:372:ASP:H	2:P:375:GLN:NE2	2.05	0.54
1:C:584:MET:HG3	1:D:73:ALA:HB2	1.88	0.54
2:M:393:ARG:HG2	2:M:461:ASP:OD2	2.07	0.54
2:P:175:GLU:HG2	2:P:179:MET:HE2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:THR:HG21	1:C:537:ILE:HD11	1.88	0.54
1:D:377:ASN:H	1:D:377:ASN:ND2	2.05	0.54
2:M:369:ILE:HG21	2:M:473:LYS:HG2	1.89	0.54
2:N:339:TYR:CD2	2:N:340:VAL:HG23	2.41	0.54
2:P:613:ILE:O	2:P:671:PRO:HD3	2.07	0.54
1:A:559:LEU:HG	1:A:563:MET:HE2	1.88	0.54
1:B:607:MET:HE2	1:B:610:VAL:CG2	2.37	0.54
1:D:559:LEU:HG	1:D:563:MET:HE3	1.89	0.54
2:N:174:LYS:NZ	2:N:174:LYS:HB3	2.22	0.54
2:N:602:MET:CE	2:N:647:ILE:HG21	2.38	0.54
2:O:266:ALA:HB1	2:O:276:VAL:HG21	1.90	0.54
1:A:377:ASN:H	1:A:377:ASN:HD22	1.55	0.54
1:B:33:VAL:HG13	1:B:339:LEU:CD1	2.38	0.54
2:M:356:VAL:HG21	2:M:361:ILE:HB	1.89	0.54
2:N:6:LYS:O	2:N:9:GLU:HB2	2.07	0.54
1:B:150:VAL:HG12	1:B:150:VAL:O	2.07	0.54
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.90	0.54
2:M:704:ILE:HD13	2:M:714:TYR:CG	2.43	0.54
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.20	0.54
2:N:602:MET:HE2	2:N:647:ILE:HG21	1.90	0.54
2:N:704:ILE:HG13	2:N:705:GLY:N	2.23	0.54
2:O:339:TYR:HB2	2:O:432:LYS:HA	1.88	0.54
2:P:424:ASN:HD22	2:P:424:ASN:N	2.05	0.54
2:P:704:ILE:HG13	2:P:705:GLY:N	2.22	0.54
1:D:118:ASN:C	1:D:118:ASN:HD22	2.16	0.54
2:M:110:ALA:CB	2:M:216:VAL:CG2	2.86	0.54
2:N:315:LYS:HB3	2:N:315:LYS:NZ	2.22	0.54
2:O:174:LYS:HB3	2:O:174:LYS:NZ	2.22	0.54
2:P:356:VAL:HG21	2:P:361:ILE:HB	1.90	0.54
1:B:377:ASN:H	1:B:377:ASN:ND2	2.05	0.54
1:B:559:LEU:HG	1:B:563:MET:HE3	1.89	0.54
2:M:342:MET:HG3	2:M:384:LEU:CD2	2.38	0.54
2:M:509:CYS:HB3	7:M:950:ACT:H1	1.89	0.53
2:O:346:ARG:HG3	2:O:346:ARG:HH11	1.72	0.53
2:O:356:VAL:HG21	2:O:361:ILE:HB	1.90	0.53
2:P:393:ARG:HG2	2:P:461:ASP:OD2	2.08	0.53
1:A:399:THR:HG22	1:A:403:MET:HE3	1.89	0.53
1:C:585:SER:OG	4:C:800:XCC:S4	2.64	0.53
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.40	0.53
1:D:607:MET:HE2	1:D:610:VAL:HG22	1.90	0.53
2:N:588:MET:HE1	2:N:604:ILE:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:373:ILE:CD1	2:O:435:VAL:HG22	2.38	0.53
2:O:469:THR:O	2:O:470:ASP:HB2	2.08	0.53
2:P:150:ASP:OD2	2:P:152:THR:HG23	2.07	0.53
2:P:722:ALA:HA	2:P:725:MET:HE3	1.88	0.53
1:B:78:ILE:HD11	1:B:97:ILE:HD12	1.89	0.53
2:N:516:HIS:HE1	2:N:518:CYS:SG	2.32	0.53
2:O:406:ARG:HB3	2:O:406:ARG:HH11	1.72	0.53
2:O:500:VAL:HG22	2:O:502:THR:H	1.72	0.53
1:A:147:CYS:SG	1:A:166:VAL:HG13	2.48	0.53
1:B:31:PRO:HB2	1:B:423:ILE:HD13	1.90	0.53
1:D:615:LEU:HD22	2:P:260:MET:SD	2.48	0.53
1:C:147:CYS:SG	1:C:166:VAL:HG13	2.48	0.53
2:M:175:GLU:HG2	2:M:179:MET:HE2	1.90	0.53
2:M:373:ILE:CD1	2:M:435:VAL:HG22	2.37	0.53
2:N:367:GLU:HG2	8:N:1215:HOH:O	2.08	0.53
2:O:372:ASP:H	2:O:375:GLN:NE2	2.06	0.53
2:O:497:ASP:O	2:O:500:VAL:O	2.26	0.53
2:M:151:TRP:CZ2	2:M:249:ARG:NH1	2.76	0.53
2:P:266:ALA:HB1	2:P:276:VAL:HG21	1.90	0.53
1:D:147:CYS:SG	1:D:166:VAL:HG13	2.49	0.53
2:M:4:PHE:HB2	2:M:238:GLU:OE2	2.09	0.53
1:C:33:VAL:HG13	1:C:339:LEU:CD1	2.39	0.53
1:D:303:LYS:HA	1:D:307:ALA:O	2.09	0.53
2:P:377:PRO:HG2	2:P:380:SER:CB	2.38	0.53
1:A:615:LEU:HD23	2:M:27:HIS:HB3	1.90	0.53
1:C:73:ALA:HB2	1:D:584:MET:HG3	1.90	0.53
1:C:607:MET:HE1	1:C:634:PHE:CD1	2.44	0.53
2:P:479:GLU:OE2	2:P:482:ARG:HD3	2.08	0.53
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.91	0.53
1:C:283:HIS:CA	1:C:318:THR:HG23	2.39	0.53
1:C:607:MET:HE2	1:C:610:VAL:CG2	2.39	0.53
1:D:33:VAL:HG13	1:D:339:LEU:HD12	1.90	0.53
2:M:613:ILE:O	2:M:671:PRO:HD3	2.09	0.53
2:N:333:ILE:HD12	2:N:431:SER:HB3	1.90	0.53
2:P:571:LEU:HD22	2:P:579:LEU:HB2	1.90	0.53
1:B:66:ILE:HG23	1:B:612:GLY:HA3	1.90	0.52
1:B:411:ARG:HG2	1:B:416:ARG:HD2	1.90	0.52
1:C:415:ASN:O	1:C:417:PRO:HD3	2.09	0.52
2:P:482:ARG:HG2	2:P:486:LYS:NZ	2.24	0.52
2:O:457:PRO:O	2:O:458:ALA:HB3	2.09	0.52
2:O:602:MET:HE2	2:O:647:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:167:LYS:HG2	8:P:1026:HOH:O	2.08	0.52
2:P:500:VAL:HG22	2:P:502:THR:H	1.72	0.52
2:P:506:CYS:HA	2:P:547:PRO:O	2.09	0.52
1:B:414:SER:O	1:B:416:ARG:N	2.43	0.52
1:C:3:ARG:HH12	1:C:625:SER:HB2	1.73	0.52
1:C:148:ARG:HB3	1:C:148:ARG:NH1	2.22	0.52
1:C:415:ASN:C	1:C:415:ASN:HD22	2.15	0.52
1:D:399:THR:HG22	1:D:403:MET:HE3	1.92	0.52
2:M:317:LYS:O	2:M:317:LYS:HG3	2.08	0.52
2:M:358:GLU:HG3	2:M:462:ARG:NH1	2.24	0.52
2:P:346:ARG:HG3	2:P:346:ARG:HH11	1.75	0.52
2:P:373:ILE:CD1	2:P:435:VAL:HG22	2.38	0.52
2:P:457:PRO:O	2:P:458:ALA:HB3	2.09	0.52
1:A:482:LEU:CD2	1:A:508:LEU:HD12	2.39	0.52
1:B:615:LEU:HD23	2:N:27:HIS:HB3	1.91	0.52
1:C:31:PRO:HB2	1:C:423:ILE:HD13	1.91	0.52
1:C:66:ILE:HG23	1:C:612:GLY:HA3	1.90	0.52
1:C:221:MET:HE2	1:D:584:MET:HE2	1.90	0.52
2:M:602:MET:CE	2:M:647:ILE:HG21	2.39	0.52
2:N:340:VAL:HG12	2:N:341:GLU:N	2.25	0.52
2:N:727:PRO:HB2	2:N:729:MET:HG3	1.89	0.52
2:O:342:MET:HG3	2:O:384:LEU:CD2	2.37	0.52
2:M:704:ILE:HG13	2:M:705:GLY:N	2.24	0.52
2:N:356:VAL:HG21	2:N:361:ILE:HB	1.92	0.52
2:P:507:VAL:HB	2:P:510:GLN:HG3	1.92	0.52
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.92	0.52
2:M:150:ASP:OD2	2:M:152:THR:HG23	2.10	0.52
2:M:186:CYS:O	2:M:187:ASP:HB2	2.10	0.52
1:A:515:ASN:HA	1:A:518:THR:HG23	1.91	0.52
2:N:377:PRO:HG2	2:N:380:SER:CB	2.39	0.52
1:B:653:THR:HG22	8:B:907:HOH:O	2.10	0.52
1:C:607:MET:HE2	1:C:610:VAL:HG22	1.91	0.52
1:D:33:VAL:HG13	1:D:339:LEU:CD1	2.40	0.52
2:P:4:PHE:HB2	2:P:238:GLU:OE2	2.09	0.52
1:D:150:VAL:HG12	1:D:150:VAL:O	2.09	0.52
1:D:415:ASN:O	1:D:417:PRO:HD3	2.09	0.52
1:D:587:LYS:HE3	4:D:800:XCC:S4	2.49	0.52
2:N:346:ARG:HG3	2:N:346:ARG:HH11	1.74	0.52
2:O:613:ILE:O	2:O:671:PRO:HD3	2.09	0.52
1:B:515:ASN:HA	1:B:518:THR:HG23	1.91	0.52
2:M:571:LEU:HD22	2:M:579:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:506:CYS:HA	2:N:547:PRO:O	2.10	0.52
2:O:507:VAL:HB	2:O:510:GLN:HG3	1.92	0.52
2:P:342:MET:HG3	2:P:384:LEU:CD2	2.38	0.52
1:C:416:ARG:HG3	1:C:416:ARG:O	2.10	0.51
2:O:377:PRO:HG2	2:O:380:SER:CB	2.37	0.51
1:B:460:GLU:CD	1:B:530:ARG:HH22	2.18	0.51
1:C:351:VAL:HG22	1:C:356:ILE:CD1	2.40	0.51
2:O:456:PHE:HD2	2:O:542:ILE:HD11	1.74	0.51
1:A:150:VAL:HG12	1:A:150:VAL:O	2.10	0.51
1:B:283:HIS:CA	1:B:318:THR:HG23	2.40	0.51
1:D:377:ASN:H	1:D:377:ASN:HD22	1.59	0.51
2:N:175:GLU:HG2	2:N:179:MET:HE2	1.91	0.51
2:O:342:MET:HB3	2:O:382:LEU:O	2.09	0.51
2:O:725:MET:O	2:O:726:ASP:HB3	2.09	0.51
2:P:61:TYR:O	2:P:63:PRO:HD3	2.10	0.51
1:D:278:PHE:HB3	1:D:312:LEU:HD23	1.92	0.51
2:M:266:ALA:HB1	2:M:276:VAL:HG21	1.91	0.51
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.91	0.51
1:A:585:SER:OG	4:A:800:XCC:S4	2.65	0.51
2:M:457:PRO:O	2:M:458:ALA:HB3	2.10	0.51
1:A:149:ARG:NH2	1:A:250:ASP:OD2	2.40	0.51
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.10	0.51
2:O:495:LEU:HD11	2:O:533:TRP:CZ3	2.46	0.51
2:P:470:ASP:OD1	2:P:472:ALA:HB3	2.10	0.51
2:P:497:ASP:OD1	2:P:522:PRO:HD2	2.11	0.51
1:C:150:VAL:HG12	1:C:150:VAL:O	2.11	0.51
2:P:340:VAL:HG12	2:P:341:GLU:N	2.26	0.51
2:P:626:MET:HB3	2:P:630:THR:HB	1.92	0.51
1:A:426:ARG:NH2	1:A:539:ILE:CG1	2.65	0.51
1:B:176:ARG:O	1:B:207:GLY:HA3	2.11	0.51
2:N:722:ALA:HA	2:N:725:MET:HE2	1.93	0.51
2:O:609:ASN:OD1	2:O:727:PRO:HA	2.10	0.51
2:O:704:ILE:HD13	2:O:714:TYR:CG	2.45	0.51
2:N:457:PRO:O	2:N:458:ALA:HB3	2.11	0.51
1:A:283:HIS:CA	1:A:318:THR:HG23	2.41	0.51
1:A:294:ALA:O	1:A:298:MET:HG2	2.10	0.51
1:A:351:VAL:HG22	1:A:356:ILE:CD1	2.40	0.51
1:A:415:ASN:HD22	1:A:415:ASN:C	2.19	0.51
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.25	0.51
1:C:335:ALA:HB2	1:C:471:ASN:HB3	1.93	0.51
2:O:495:LEU:HD21	2:O:533:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:704:ILE:HG13	2:O:705:GLY:N	2.25	0.51
2:M:346:ARG:HG3	2:M:346:ARG:HH11	1.75	0.50
1:A:24:ASN:O	1:A:27:ARG:HG2	2.11	0.50
1:C:24:ASN:O	1:C:27:ARG:HG2	2.12	0.50
1:D:61:ILE:HD13	1:D:77:ARG:HE	1.76	0.50
2:M:506:CYS:HA	2:M:547:PRO:O	2.10	0.50
2:N:722:ALA:HA	2:N:725:MET:CE	2.40	0.50
2:O:482:ARG:HA	2:O:482:ARG:CZ	2.41	0.50
2:M:602:MET:HE2	2:M:647:ILE:HG21	1.93	0.50
2:P:174:LYS:NZ	2:P:174:LYS:HB3	2.27	0.50
2:P:406:ARG:HB3	2:P:406:ARG:HH11	1.76	0.50
2:M:340:VAL:HG12	2:M:341:GLU:N	2.26	0.50
2:O:626:MET:HB3	2:O:630:THR:HB	1.93	0.50
1:A:105:MET:HE1	1:A:609:PRO:HD2	1.93	0.50
1:C:18:ARG:NE	1:C:636:MET:HE3	2.26	0.50
2:M:19:VAL:HG23	2:M:20:ALA:N	2.27	0.50
2:N:350:PHE:CD1	2:N:350:PHE:C	2.90	0.50
2:N:604:ILE:HD12	2:N:604:ILE:O	2.11	0.50
2:P:224:ARG:O	2:P:228:MET:HG3	2.11	0.50
1:D:66:ILE:HG23	1:D:612:GLY:HA3	1.93	0.50
1:A:73:ALA:HB2	1:B:584:MET:HG3	1.94	0.50
1:A:278:PHE:HB3	1:A:312:LEU:HD23	1.94	0.50
2:O:186:CYS:O	2:O:187:ASP:HB2	2.12	0.50
2:O:339:TYR:CG	2:O:435:VAL:HG21	2.47	0.50
2:O:471:GLU:O	2:O:475:LYS:HG2	2.11	0.50
2:O:496:THR:HG1	2:O:499:THR:H	1.59	0.50
1:C:280:LEU:HD13	1:C:288:SER:HB2	1.94	0.50
1:D:283:HIS:CA	1:D:318:THR:HG23	2.42	0.50
1:D:335:ALA:HB2	1:D:471:ASN:HB3	1.92	0.50
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.47	0.50
2:N:354:ARG:HD2	2:N:389:ASP:OD2	2.12	0.50
2:O:340:VAL:HG12	2:O:341:GLU:N	2.27	0.50
2:O:564:TRP:CZ3	2:O:584:LEU:HD12	2.47	0.50
1:B:3:ARG:CG	1:B:3:ARG:NH2	2.70	0.50
2:M:482:ARG:HG2	2:M:486:LYS:NZ	2.27	0.50
2:M:505:SER:HB3	2:M:551:ILE:HD11	1.94	0.50
2:O:114:GLU:OE1	2:O:117:ARG:NH1	2.45	0.50
1:B:377:ASN:H	1:B:377:ASN:HD22	1.58	0.49
1:C:487:GLU:HB2	8:C:907:HOH:O	2.11	0.49
2:M:707:THR:OG1	2:M:710:GLU:HG3	2.12	0.49
1:B:150:VAL:HG13	1:B:184:THR:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.94	0.49
1:D:607:MET:HE2	1:D:610:VAL:CG2	2.41	0.49
2:M:439:PHE:C	2:M:440:ARG:HD2	2.37	0.49
2:N:372:ASP:OD1	2:N:373:ILE:N	2.41	0.49
1:A:31:PRO:HB2	1:A:423:ILE:HD13	1.93	0.49
1:A:587:LYS:HE3	4:A:800:XCC:S4	2.52	0.49
1:B:351:VAL:HG21	1:B:356:ILE:HG12	1.93	0.49
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.42	0.49
1:C:510:LEU:O	1:C:543:PRO:HD2	2.13	0.49
2:M:622:THR:HB	2:M:623:PRO:HD2	1.95	0.49
2:N:342:MET:HG3	2:N:384:LEU:CD2	2.40	0.49
2:N:587:LEU:HD23	2:N:588:MET:HE1	1.93	0.49
1:A:150:VAL:HG13	1:A:184:THR:HG21	1.93	0.49
2:M:395:MET:HE3	2:M:396:GLN:O	2.12	0.49
2:M:568:ASN:OD1	2:M:581:GLN:HG3	2.12	0.49
2:O:445:GLY:O	2:O:449:VAL:HG23	2.12	0.49
1:C:176:ARG:O	1:C:207:GLY:HA3	2.13	0.49
1:C:525:LYS:O	1:C:529:LYS:HG2	2.13	0.49
2:M:393:ARG:HG3	2:M:393:ARG:HH11	1.78	0.49
2:N:613:ILE:O	2:N:671:PRO:HD3	2.12	0.49
2:O:700:ALA:CB	2:O:704:ILE:HD11	2.43	0.49
1:A:655:LYS:HG3	2:M:191:GLU:HG2	1.94	0.49
2:P:473:LYS:HA	2:P:476:GLU:HB3	1.94	0.49
1:A:656:LEU:O	1:A:660:LYS:HG3	2.13	0.49
2:N:439:PHE:C	2:N:440:ARG:HD2	2.38	0.49
2:O:439:PHE:C	2:O:440:ARG:HD2	2.37	0.49
1:B:278:PHE:HB3	1:B:312:LEU:HD23	1.94	0.49
1:B:282:GLY:C	1:B:318:THR:HG23	2.38	0.49
1:B:653:THR:CG2	8:B:907:HOH:O	2.61	0.49
1:C:313:VAL:CB	1:C:331:VAL:HG22	2.38	0.49
1:D:313:VAL:CB	1:D:331:VAL:HG22	2.38	0.49
2:N:666:ARG:HD3	2:N:725:MET:HE3	1.94	0.49
1:B:150:VAL:O	1:B:150:VAL:CG1	2.61	0.49
2:P:707:THR:OG1	2:P:710:GLU:HG3	2.12	0.49
1:B:68:CYS:HB2	1:B:97:ILE:HG23	1.96	0.48
1:D:24:ASN:O	1:D:27:ARG:HG2	2.13	0.48
2:M:424:ASN:HD22	2:M:424:ASN:N	2.05	0.48
1:B:125:VAL:O	1:B:129:GLU:HG3	2.13	0.48
2:N:626:MET:HB3	2:N:630:THR:HB	1.95	0.48
2:O:602:MET:CE	2:O:647:ILE:HG21	2.43	0.48
2:P:210:GLY:HA3	2:P:214:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:350:PHE:CD1	2:P:350:PHE:C	2.90	0.48
1:A:105:MET:CE	1:A:609:PRO:HD2	2.43	0.48
1:B:399:THR:HG22	1:B:403:MET:HE3	1.96	0.48
2:O:348:PRO:HB3	2:O:475:LYS:HZ1	1.77	0.48
2:O:707:THR:OG1	2:O:710:GLU:HG3	2.13	0.48
2:P:505:SER:HB3	2:P:551:ILE:HD11	1.95	0.48
2:O:568:ASN:CG	2:O:581:GLN:HG3	2.38	0.48
2:O:712:LEU:N	2:O:713:PRO:HD2	2.29	0.48
2:P:13:PRO:HB2	2:P:16:LYS:HG3	1.94	0.48
1:A:68:CYS:HB2	1:A:97:ILE:HG23	1.96	0.48
1:D:409:LYS:O	1:D:413:GLU:HG2	2.14	0.48
1:D:530:ARG:NH1	1:D:530:ARG:HB2	2.29	0.48
2:P:66:ARG:O	2:P:70:GLY:HA2	2.14	0.48
1:B:24:ASN:O	1:B:27:ARG:HG2	2.14	0.48
1:D:480:SER:HB2	1:D:582:GLU:HG3	1.94	0.48
2:M:670:MET:HE2	2:M:699:ILE:HD13	1.96	0.48
2:N:497:ASP:H	2:N:523:GLU:CD	2.18	0.48
2:O:314:THR:O	2:O:315:LYS:C	2.56	0.48
2:P:439:PHE:C	2:P:440:ARG:HD2	2.38	0.48
2:P:704:ILE:HD13	2:P:714:TYR:CG	2.49	0.48
1:A:577:VAL:HG21	1:A:645:ILE:CG2	2.41	0.48
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.29	0.48
2:M:339:TYR:CG	2:M:435:VAL:HG21	2.49	0.48
2:N:424:ASN:HD22	2:N:424:ASN:N	2.05	0.48
2:N:568:ASN:OD1	2:N:581:GLN:HG3	2.14	0.48
2:O:19:VAL:HG23	2:O:20:ALA:N	2.28	0.48
1:C:377:ASN:HD22	1:C:377:ASN:N	2.05	0.48
1:D:150:VAL:HG13	1:D:184:THR:HG21	1.96	0.48
1:D:559:LEU:HG	1:D:563:MET:HE2	1.95	0.48
2:M:71:GLU:H	2:M:71:GLU:CD	2.22	0.48
2:M:377:PRO:HG2	2:M:380:SER:CB	2.40	0.48
2:N:61:TYR:O	2:N:63:PRO:HD3	2.14	0.48
2:P:376:ILE:HD12	2:P:376:ILE:C	2.38	0.48
1:A:335:ALA:HB2	1:A:471:ASN:HB3	1.96	0.48
1:A:351:VAL:HG21	1:A:356:ILE:HG12	1.95	0.48
1:A:412:LYS:HA	1:A:416:ARG:HD3	1.96	0.48
1:B:335:ALA:HB2	1:B:471:ASN:HB3	1.96	0.48
1:B:577:VAL:HG21	1:B:645:ILE:CG2	2.40	0.48
1:C:150:VAL:HG13	1:C:184:THR:HG21	1.96	0.48
2:N:266:ALA:HB1	2:N:276:VAL:HG21	1.96	0.48
2:P:602:MET:CE	2:P:647:ILE:HG21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:VAL:HG22	1:D:356:ILE:CD1	2.44	0.48
2:M:588:MET:HE3	2:M:728:ILE:HD11	1.96	0.48
2:M:712:LEU:N	2:M:713:PRO:HD2	2.28	0.48
2:N:479:GLU:HA	2:N:482:ARG:HG3	1.96	0.48
2:O:604:ILE:HD13	2:O:606:PRO:HD3	1.96	0.48
2:O:622:THR:HB	2:O:623:PRO:HD2	1.96	0.48
1:B:318:THR:HG21	8:B:855:HOH:O	2.14	0.47
1:B:615:LEU:CD2	2:N:27:HIS:HB3	2.44	0.47
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.47	0.47
1:D:525:LYS:O	1:D:529:LYS:HG2	2.14	0.47
2:N:670:MET:HE2	2:N:699:ILE:HD13	1.96	0.47
1:A:176:ARG:O	1:A:207:GLY:HA3	2.13	0.47
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.45	0.47
2:M:350:PHE:CD1	2:M:350:PHE:C	2.92	0.47
2:N:19:VAL:HG22	8:N:1251:HOH:O	2.14	0.47
2:N:406:ARG:HB3	2:N:406:ARG:HH11	1.78	0.47
2:P:604:ILE:HD13	2:P:606:PRO:HD3	1.96	0.47
2:M:657:PHE:O	2:M:658:ILE:C	2.57	0.47
2:O:376:ILE:C	2:O:376:ILE:HD12	2.40	0.47
2:O:496:THR:O	2:O:500:VAL:HG12	2.15	0.47
2:O:568:ASN:OD1	2:O:581:GLN:HG3	2.14	0.47
2:P:712:LEU:N	2:P:713:PRO:HD2	2.28	0.47
1:A:282:GLY:C	1:A:318:THR:HG23	2.38	0.47
1:A:525:LYS:O	1:A:529:LYS:HG2	2.15	0.47
1:C:581:PRO:O	1:C:605:GLY:HA3	2.14	0.47
1:C:656:LEU:O	1:C:660:LYS:HG3	2.14	0.47
2:M:468:PHE:CD2	2:M:473:LYS:HG3	2.50	0.47
2:N:564:TRP:CZ3	2:N:584:LEU:HD12	2.48	0.47
2:O:410:PHE:CZ	2:O:455:GLU:HG3	2.50	0.47
2:P:657:PHE:O	2:P:658:ILE:C	2.57	0.47
1:B:607:MET:HE2	1:B:610:VAL:HG22	1.96	0.47
1:C:61:ILE:HD13	1:C:77:ARG:HE	1.78	0.47
2:O:371:PRO:HD2	2:O:469:THR:O	2.14	0.47
2:O:665:ALA:O	2:O:722:ALA:HB2	2.14	0.47
1:A:510:LEU:O	1:A:543:PRO:HD2	2.15	0.47
1:B:615:LEU:HD23	2:N:27:HIS:CB	2.44	0.47
1:C:105:MET:CE	1:C:609:PRO:HD2	2.45	0.47
1:D:3:ARG:NH2	1:D:625:SER:CB	2.75	0.47
1:D:154:VAL:HG13	1:D:162:LEU:HD11	1.97	0.47
2:M:597:CYS:HB3	7:M:950:ACT:O	2.14	0.47
2:N:186:CYS:O	2:N:187:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:342:MET:SD	2:N:342:MET:N	2.88	0.47
2:O:657:PHE:O	2:O:658:ILE:C	2.56	0.47
1:B:150:VAL:CG1	1:B:169:LYS:HG2	2.40	0.47
1:B:655:LYS:HG3	2:N:191:GLU:HG2	1.96	0.47
1:C:559:LEU:HG	1:C:563:MET:HE2	1.97	0.47
1:D:18:ARG:NE	1:D:636:MET:HE3	2.29	0.47
2:M:626:MET:HB3	2:M:630:THR:HB	1.97	0.47
2:O:505:SER:HB3	2:O:551:ILE:HD11	1.95	0.47
2:P:445:GLY:O	2:P:449:VAL:HG23	2.14	0.47
2:P:564:TRP:CZ3	2:P:584:LEU:HD12	2.50	0.47
1:A:318:THR:O	1:A:322:VAL:HG22	2.15	0.47
1:C:394:ILE:HG23	1:C:395:GLU:N	2.30	0.47
2:N:393:ARG:HH11	2:N:393:ARG:HG3	1.80	0.47
2:P:138:ASP:N	2:P:139:PRO:CD	2.77	0.47
1:B:443:GLN:HB2	1:B:451:VAL:HG21	1.96	0.47
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.50	0.47
2:N:712:LEU:N	2:N:713:PRO:HD2	2.30	0.47
2:O:350:PHE:CD1	2:O:350:PHE:C	2.92	0.47
2:P:393:ARG:HG3	2:P:393:ARG:HH11	1.78	0.47
1:B:190:ILE:HG13	1:B:195:LYS:HG3	1.97	0.47
1:B:307:ALA:HB2	1:B:408:PHE:CE2	2.49	0.47
1:B:587:LYS:HE3	4:B:800:XCC:S4	2.55	0.47
1:C:577:VAL:HG21	1:C:645:ILE:CG2	2.43	0.47
1:D:176:ARG:O	1:D:207:GLY:HA3	2.15	0.47
1:D:190:ILE:HG13	1:D:195:LYS:HG3	1.97	0.47
2:N:354:ARG:NH2	2:N:480:VAL:HG11	2.27	0.47
1:A:443:GLN:HB2	1:A:451:VAL:HG21	1.96	0.46
2:O:356:VAL:CG2	2:O:361:ILE:HB	2.45	0.46
2:O:670:MET:HE2	2:O:699:ILE:HD13	1.96	0.46
2:P:622:THR:HB	2:P:623:PRO:HD2	1.96	0.46
1:A:615:LEU:CD2	2:M:27:HIS:HB3	2.46	0.46
1:C:615:LEU:HD13	1:C:615:LEU:C	2.40	0.46
1:D:601:PRO:HD3	1:D:652:ARG:CZ	2.45	0.46
2:M:507:VAL:HB	2:M:510:GLN:HG3	1.97	0.46
2:N:314:THR:O	2:N:315:LYS:C	2.58	0.46
2:P:470:ASP:O	2:P:474:VAL:HG23	2.16	0.46
2:P:722:ALA:HA	2:P:725:MET:HE2	1.97	0.46
1:B:412:LYS:NZ	1:B:416:ARG:CZ	2.79	0.46
1:C:377:ASN:HB2	1:D:218:GLN:HG3	1.97	0.46
1:C:480:SER:HB2	1:C:582:GLU:HG3	1.96	0.46
1:D:469:GLY:O	4:D:800:XCC:S1	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:372:ASP:OD1	2:M:373:ILE:N	2.41	0.46
2:N:138:ASP:N	2:N:139:PRO:CD	2.79	0.46
2:N:376:ILE:HD12	2:N:376:ILE:C	2.41	0.46
2:P:372:ASP:OD1	2:P:373:ILE:N	2.43	0.46
1:C:584:MET:HE2	1:D:221:MET:HE2	1.97	0.46
2:M:352:LEU:HD22	2:M:481:ALA:HB2	1.98	0.46
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.14	0.46
2:P:114:GLU:OE1	2:P:117:ARG:NH1	2.48	0.46
2:P:568:ASN:CG	2:P:581:GLN:HG3	2.41	0.46
1:A:480:SER:HB2	1:A:582:GLU:HG3	1.97	0.46
1:A:486:LYS:HE2	1:A:519:TYR:CE2	2.50	0.46
2:N:586:THR:HG22	2:N:587:LEU:N	2.30	0.46
2:O:138:ASP:N	2:O:139:PRO:CD	2.77	0.46
2:O:247:ARG:HB3	2:O:512:PHE:CE2	2.51	0.46
2:O:371:PRO:HD2	2:O:469:THR:OG1	2.16	0.46
2:O:424:ASN:HD22	2:O:424:ASN:N	2.06	0.46
2:P:365:LYS:HE2	2:P:367:GLU:OE2	2.15	0.46
2:P:410:PHE:CZ	2:P:455:GLU:HG3	2.50	0.46
2:P:419:HIS:HB2	2:P:428:LEU:HD13	1.97	0.46
2:P:482:ARG:HG2	2:P:486:LYS:HZ1	1.81	0.46
2:P:568:ASN:OD1	2:P:581:GLN:HG3	2.16	0.46
1:B:61:ILE:HD13	1:B:77:ARG:HE	1.81	0.46
1:C:190:ILE:HG13	1:C:195:LYS:HG3	1.97	0.46
1:C:615:LEU:HD22	2:O:260:MET:SD	2.55	0.46
2:M:365:LYS:HE2	2:M:367:GLU:OE2	2.15	0.46
2:M:406:ARG:HB3	2:M:406:ARG:HH11	1.79	0.46
2:M:445:GLY:O	2:M:449:VAL:HG23	2.15	0.46
2:O:66:ARG:O	2:O:70:GLY:HA2	2.15	0.46
2:O:318:LEU:HD12	2:O:318:LEU:O	2.16	0.46
2:O:367:GLU:HG3	2:O:466:THR:HG23	1.97	0.46
2:P:186:CYS:O	2:P:187:ASP:HB2	2.15	0.46
1:A:559:LEU:HG	1:A:563:MET:HE3	1.97	0.46
1:D:656:LEU:O	1:D:660:LYS:HG3	2.16	0.46
2:M:66:ARG:O	2:M:70:GLY:HA2	2.15	0.46
2:O:419:HIS:HB2	2:O:428:LEU:HD13	1.98	0.46
2:O:478:MET:HE3	2:O:478:MET:HA	1.98	0.46
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.41	0.46
1:B:411:ARG:CG	1:B:416:ARG:HD2	2.46	0.46
2:M:356:VAL:CG2	2:M:361:ILE:HB	2.45	0.46
2:M:376:ILE:C	2:M:376:ILE:HD12	2.41	0.46
2:M:419:HIS:ND1	2:M:419:HIS:C	2.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:586:THR:HG22	2:M:587:LEU:N	2.31	0.46
2:O:210:GLY:HA3	2:O:214:GLN:HE21	1.81	0.46
2:O:586:THR:HG22	2:O:587:LEU:N	2.31	0.46
1:A:415:ASN:O	1:A:417:PRO:CD	2.64	0.46
1:C:559:LEU:HG	1:C:563:MET:HE3	1.97	0.46
1:D:105:MET:CE	1:D:609:PRO:HD2	2.46	0.46
2:M:439:PHE:CE1	2:M:443:ASN:HB2	2.51	0.46
2:P:247:ARG:HB3	2:P:512:PHE:CE2	2.51	0.46
1:B:581:PRO:O	1:B:605:GLY:HA3	2.16	0.45
1:C:78:ILE:HD11	1:C:97:ILE:HD12	1.98	0.45
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.46	0.45
1:D:662:VAL:HG21	2:P:194:LEU:HD13	1.97	0.45
2:M:124:ASP:OD1	2:M:125:GLU:HG3	2.16	0.45
2:M:568:ASN:CG	2:M:581:GLN:HG3	2.41	0.45
2:N:622:THR:HB	2:N:623:PRO:HD2	1.98	0.45
2:O:381:LYS:O	2:O:382:LEU:HB2	2.16	0.45
2:O:497:ASP:HA	2:O:500:VAL:CG1	2.43	0.45
2:O:680:ASP:O	2:O:684:ARG:HG3	2.16	0.45
2:P:609:ASN:OD1	2:P:728:ILE:HG22	2.16	0.45
1:B:525:LYS:O	1:B:529:LYS:HG2	2.16	0.45
1:C:149:ARG:NH2	1:C:250:ASP:OD2	2.45	0.45
1:D:150:VAL:O	1:D:150:VAL:CG1	2.64	0.45
2:N:66:ARG:HD3	8:N:1160:HOH:O	2.16	0.45
2:O:372:ASP:OD1	2:O:373:ILE:N	2.42	0.45
2:P:680:ASP:O	2:P:684:ARG:HG3	2.16	0.45
1:B:105:MET:CE	1:B:609:PRO:HD2	2.46	0.45
1:C:569:VAL:HB	1:C:573:LYS:HD3	1.97	0.45
2:P:71:GLU:H	2:P:71:GLU:CD	2.23	0.45
1:A:571:THR:OG1	1:A:572:PRO:HD3	2.16	0.45
1:A:615:LEU:HD23	2:M:27:HIS:CB	2.47	0.45
1:B:415:ASN:O	1:B:417:PRO:CD	2.63	0.45
2:M:199:LYS:CA	2:M:199:LYS:HE2	2.47	0.45
2:M:726:ASP:HB2	2:M:727:PRO:HD2	1.97	0.45
2:O:376:ILE:HD12	2:O:376:ILE:O	2.17	0.45
2:O:564:TRP:HZ3	2:O:584:LEU:HD12	1.81	0.45
2:P:496:THR:O	2:P:500:VAL:N	2.49	0.45
1:A:468:CYS:HB2	8:A:803:HOH:O	2.16	0.45
1:C:399:THR:HG22	1:C:403:MET:HE3	1.99	0.45
2:M:564:TRP:CZ3	2:M:584:LEU:HD12	2.52	0.45
2:N:356:VAL:CG2	2:N:361:ILE:HB	2.46	0.45
2:O:419:HIS:ND1	2:O:419:HIS:C	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:475:LYS:HA	2:O:478:MET:CB	2.44	0.45
2:P:339:TYR:CG	2:P:435:VAL:HG21	2.52	0.45
2:P:356:VAL:CG2	2:P:361:ILE:HB	2.45	0.45
2:P:419:HIS:ND1	2:P:419:HIS:C	2.74	0.45
1:A:313:VAL:CB	1:A:331:VAL:HG22	2.37	0.45
1:B:480:SER:HB2	1:B:582:GLU:HG3	1.99	0.45
1:C:153:GLU:O	1:C:157:LYS:HD2	2.17	0.45
1:D:3:ARG:O	2:P:162:ARG:NH1	2.49	0.45
1:D:150:VAL:CG1	1:D:169:LYS:HE2	2.46	0.45
2:M:151:TRP:CE3	2:M:249:ARG:NH1	2.84	0.45
2:M:367:GLU:HG3	2:M:466:THR:HG23	1.97	0.45
2:M:419:HIS:HB2	2:M:428:LEU:HD13	1.98	0.45
2:N:71:GLU:H	2:N:71:GLU:CD	2.25	0.45
2:P:376:ILE:HD12	2:P:376:ILE:O	2.16	0.45
2:P:473:LYS:HG2	2:P:476:GLU:OE2	2.17	0.45
1:B:273:PRO:HB2	1:B:416:ARG:HH21	1.82	0.45
1:D:125:VAL:O	1:D:129:GLU:HG3	2.16	0.45
2:N:586:THR:HG23	2:N:661:ASP:OD1	2.17	0.45
1:B:18:ARG:NE	1:B:636:MET:HE3	2.32	0.45
1:C:466:LEU:HD22	1:C:595:TRP:CZ2	2.51	0.45
1:D:581:PRO:O	1:D:605:GLY:HA3	2.17	0.45
2:M:410:PHE:CZ	2:M:455:GLU:HG3	2.52	0.45
2:N:381:LYS:O	2:N:382:LEU:HB2	2.17	0.45
2:P:586:THR:HG22	2:P:587:LEU:N	2.32	0.45
1:A:581:PRO:O	1:A:605:GLY:HA3	2.17	0.45
1:B:510:LEU:O	1:B:543:PRO:HD2	2.17	0.45
1:C:125:VAL:O	1:C:129:GLU:HG3	2.16	0.45
1:D:412:LYS:HD3	1:D:416:ARG:CD	2.47	0.45
1:A:150:VAL:O	1:A:150:VAL:CG1	2.65	0.45
1:A:235:ILE:HG23	1:A:597:SER:OG	2.17	0.45
1:B:569:VAL:HB	1:B:573:LYS:HD3	1.99	0.45
1:C:318:THR:O	1:C:322:VAL:HG22	2.17	0.45
1:C:415:ASN:C	1:C:415:ASN:ND2	2.74	0.45
1:D:411:ARG:O	1:D:416:ARG:HB3	2.17	0.45
2:O:365:LYS:HE2	2:O:367:GLU:OE2	2.16	0.45
1:A:3:ARG:HG2	1:A:3:ARG:NH1	2.32	0.44
1:A:394:ILE:HG23	1:A:395:GLU:N	2.33	0.44
1:B:3:ARG:NH1	1:B:625:SER:HB3	2.31	0.44
1:B:486:LYS:HE2	1:B:519:TYR:CE2	2.52	0.44
1:C:150:VAL:O	1:C:150:VAL:CG1	2.65	0.44
1:D:235:ILE:HG23	1:D:597:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:382:LEU:HD12	2:N:383:PRO:HD2	1.99	0.44
2:O:3:ASP:O	2:O:6:LYS:HG2	2.17	0.44
1:A:150:VAL:CG1	1:A:169:LYS:HG2	2.41	0.44
1:C:439:LEU:CD1	1:C:537:ILE:HD13	2.47	0.44
1:D:3:ARG:HH22	1:D:625:SER:HB2	1.78	0.44
2:N:210:GLY:HA3	2:N:214:GLN:HE21	1.81	0.44
2:N:410:PHE:CZ	2:N:455:GLU:HG3	2.52	0.44
2:P:496:THR:H	2:P:499:THR:HG1	1.62	0.44
1:A:658:VAL:O	1:A:662:VAL:HG23	2.18	0.44
2:M:114:GLU:OE1	2:M:117:ARG:NH1	2.51	0.44
2:N:114:GLU:OE1	2:N:117:ARG:NH1	2.50	0.44
2:N:456:PHE:HA	2:N:542:ILE:HD13	1.99	0.44
2:N:505:SER:HB3	2:N:551:ILE:HD11	2.00	0.44
2:N:657:PHE:O	2:N:658:ILE:C	2.59	0.44
1:A:125:VAL:O	1:A:129:GLU:HG3	2.18	0.44
1:D:486:LYS:HE2	1:D:519:TYR:CE2	2.53	0.44
2:M:138:ASP:N	2:M:139:PRO:CD	2.79	0.44
2:M:224:ARG:O	2:M:228:MET:HG3	2.17	0.44
2:N:66:ARG:O	2:N:70:GLY:HA2	2.17	0.44
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.52	0.44
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.53	0.44
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.53	0.44
1:D:150:VAL:CG1	1:D:169:LYS:HG2	2.42	0.44
1:D:318:THR:O	1:D:322:VAL:HG22	2.17	0.44
1:D:615:LEU:C	1:D:615:LEU:HD13	2.43	0.44
2:M:604:ILE:HD13	2:M:606:PRO:HD3	2.00	0.44
2:O:666:ARG:CZ	2:O:728:ILE:HB	2.48	0.44
2:P:199:LYS:CA	2:P:199:LYS:HE2	2.47	0.44
2:P:354:ARG:HD2	2:P:389:ASP:OD2	2.18	0.44
2:P:363:ASP:OD1	2:P:462:ARG:HA	2.18	0.44
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.82	0.44
1:A:652:ARG:O	1:A:656:LEU:HB2	2.18	0.44
2:O:393:ARG:HG3	2:O:393:ARG:HH11	1.82	0.44
1:A:411:ARG:CG	1:A:416:ARG:HD2	2.47	0.44
1:A:483:THR:HG23	1:A:639:GLN:HE21	1.82	0.44
1:C:150:VAL:CG1	1:C:169:LYS:HE2	2.47	0.44
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.48	0.44
2:N:568:ASN:CG	2:N:581:GLN:HG3	2.42	0.44
2:O:14:GLU:OE1	2:O:15:GLY:N	2.50	0.44
2:O:342:MET:SD	2:O:342:MET:N	2.91	0.44
2:P:199:LYS:HE2	2:P:199:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NE	1:A:636:MET:HE3	2.33	0.44
1:D:238:ALA:O	1:D:241:ASP:HB3	2.18	0.44
2:N:604:ILE:CD1	2:N:604:ILE:C	2.91	0.44
2:O:382:LEU:HD12	2:O:383:PRO:HD2	1.99	0.44
2:P:352:LEU:HD22	2:P:481:ALA:CB	2.47	0.44
1:B:150:VAL:CG1	1:B:169:LYS:HE2	2.48	0.44
1:B:656:LEU:O	1:B:660:LYS:HG3	2.16	0.44
1:C:52:PHE:CZ	1:C:474:LYS:HA	2.52	0.44
2:M:2:THR:HB	2:M:238:GLU:OE1	2.18	0.44
2:M:210:GLY:HA3	2:M:214:GLN:HE21	1.82	0.44
2:N:224:ARG:O	2:N:228:MET:HG3	2.16	0.44
1:A:61:ILE:HD13	1:A:77:ARG:HE	1.82	0.43
2:P:151:TRP:C	2:P:153:ILE:N	2.75	0.43
2:P:339:TYR:CD1	2:P:378:GLU:HG3	2.53	0.43
1:B:3:ARG:HD3	1:B:4:PHE:CE1	2.54	0.43
1:B:273:PRO:HB2	1:B:416:ARG:NH2	2.33	0.43
1:C:351:VAL:HG21	1:C:356:ILE:HG12	1.99	0.43
2:M:381:LYS:O	2:M:382:LEU:HB2	2.17	0.43
2:O:410:PHE:CE1	2:O:455:GLU:HG3	2.53	0.43
2:P:670:MET:HE2	2:P:699:ILE:HD13	1.98	0.43
1:B:394:ILE:HG23	1:B:395:GLU:N	2.34	0.43
1:C:159:VAL:HG23	1:C:160:LEU:N	2.33	0.43
1:D:510:LEU:O	1:D:543:PRO:HD2	2.18	0.43
2:N:199:LYS:CA	2:N:199:LYS:HE2	2.48	0.43
2:P:382:LEU:HD12	2:P:383:PRO:HD2	2.00	0.43
1:A:223:MET:SD	1:B:353:VAL:HB	2.59	0.43
1:A:280:LEU:HD13	1:A:288:SER:HB2	1.99	0.43
1:B:298:MET:HE1	1:B:402:ARG:CG	2.47	0.43
1:B:313:VAL:CB	1:B:331:VAL:HG22	2.38	0.43
1:B:410:GLU:HA	1:B:413:GLU:HG2	2.00	0.43
1:C:218:GLN:HG3	1:D:377:ASN:HB2	1.99	0.43
2:M:315:LYS:O	2:M:317:LYS:N	2.50	0.43
2:N:124:ASP:OD1	2:N:125:GLU:HG3	2.18	0.43
2:N:365:LYS:HE2	2:N:367:GLU:OE2	2.18	0.43
2:N:419:HIS:ND1	2:N:419:HIS:C	2.75	0.43
1:A:377:ASN:HD22	1:A:377:ASN:N	2.14	0.43
1:B:615:LEU:C	1:B:615:LEU:HD13	2.44	0.43
1:C:150:VAL:CG1	1:C:169:LYS:HG2	2.43	0.43
1:C:384:TYR:HE2	2:P:88:ALA:CB	2.31	0.43
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.53	0.43
2:M:151:TRP:CE2	2:M:249:ARG:NH1	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:399:PHE:O	2:P:403:LEU:HD13	2.19	0.43
1:D:577:VAL:HG21	1:D:645:ILE:CG2	2.45	0.43
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.54	0.43
2:N:571:LEU:HD21	2:N:579:LEU:HD12	1.99	0.43
2:O:482:ARG:HG3	2:O:486:LYS:NZ	2.33	0.43
2:P:666:ARG:NH1	2:P:728:ILE:HB	2.34	0.43
1:A:158:SER:OG	1:A:161:GLU:HG3	2.18	0.43
1:A:305:ALA:CB	1:A:409:LYS:HE3	2.49	0.43
1:D:280:LEU:HD13	1:D:288:SER:HB2	2.00	0.43
2:N:419:HIS:HB2	2:N:428:LEU:HD13	2.01	0.43
1:A:150:VAL:CG1	1:A:169:LYS:HE2	2.48	0.43
1:A:299:GLU:O	1:A:303:LYS:HG3	2.19	0.43
1:A:317:CYS:O	1:A:321:GLU:HG2	2.19	0.43
1:B:105:MET:HE1	1:B:609:PRO:HD2	2.01	0.43
2:M:199:LYS:HE2	2:M:199:LYS:N	2.34	0.43
2:M:316:ILE:O	2:M:316:ILE:HG22	2.19	0.43
1:D:569:VAL:HB	1:D:573:LYS:HD3	2.01	0.43
2:M:313:LEU:HD12	2:M:313:LEU:C	2.44	0.43
2:O:604:ILE:CD1	2:O:606:PRO:HD3	2.48	0.43
2:P:342:MET:SD	2:P:342:MET:N	2.92	0.43
2:P:595:CYS:HB2	7:P:950:ACT:H1	1.99	0.43
1:B:267:ASN:O	1:B:270:VAL:HG22	2.19	0.43
1:B:647:ASP:HB3	8:B:862:HOH:O	2.19	0.43
1:C:223:MET:SD	1:D:353:VAL:HB	2.59	0.43
1:C:443:GLN:HB2	1:C:451:VAL:HG21	2.01	0.43
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.53	0.43
2:N:238:GLU:HG2	8:N:1293:HOH:O	2.19	0.43
2:N:339:TYR:CD1	2:N:378:GLU:HG3	2.54	0.43
2:N:680:ASP:O	2:N:684:ARG:HG3	2.18	0.43
2:O:571:LEU:HD21	2:O:579:LEU:HD12	2.01	0.43
1:B:98:VAL:HG13	1:B:610:VAL:HA	2.01	0.42
1:C:352:ASP:OD1	1:C:353:VAL:N	2.43	0.42
1:C:466:LEU:HD22	1:C:595:TRP:HZ2	1.84	0.42
2:O:406:ARG:HH11	2:O:406:ARG:CB	2.32	0.42
2:O:727:PRO:C	2:O:729:MET:H	2.27	0.42
2:P:367:GLU:HG3	2:P:466:THR:HG23	2.00	0.42
1:A:377:ASN:ND2	1:A:377:ASN:N	2.64	0.42
1:A:411:ARG:HG2	1:A:416:ARG:HD2	2.01	0.42
1:D:127:MET:SD	1:D:127:MET:C	3.01	0.42
2:N:666:ARG:HD3	2:N:725:MET:CE	2.48	0.42
2:O:587:LEU:HD23	2:O:588:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ALA:O	1:B:241:ASP:HB3	2.19	0.42
1:B:241:ASP:OD2	1:B:245:GLU:OE2	2.37	0.42
1:B:351:VAL:CG2	1:B:356:ILE:CD1	2.98	0.42
1:C:326:GLN:HB2	1:C:328:ILE:HG12	2.00	0.42
1:C:652:ARG:O	1:C:656:LEU:HB2	2.19	0.42
1:D:78:ILE:HD11	1:D:97:ILE:HD12	2.02	0.42
1:D:412:LYS:C	1:D:414:SER:H	2.28	0.42
2:M:723:LEU:N	2:M:723:LEU:HD12	2.34	0.42
2:O:199:LYS:HE2	2:O:199:LYS:CA	2.49	0.42
1:A:190:ILE:HG13	1:A:195:LYS:HG3	2.00	0.42
1:A:377:ASN:HB2	1:B:218:GLN:HG3	2.01	0.42
1:C:411:ARG:HH11	1:C:416:ARG:HD2	1.83	0.42
1:D:52:PHE:CZ	1:D:474:LYS:HA	2.54	0.42
1:D:326:GLN:HB2	1:D:328:ILE:HG12	2.02	0.42
2:O:86:LYS:HA	2:O:86:LYS:HD3	1.86	0.42
2:O:439:PHE:CE1	2:O:443:ASN:HB2	2.53	0.42
2:P:381:LYS:O	2:P:382:LEU:HB2	2.19	0.42
2:P:704:ILE:HD13	2:P:714:TYR:CD2	2.54	0.42
1:C:317:CYS:O	1:C:321:GLU:HG2	2.19	0.42
1:D:416:ARG:O	1:D:418:VAL:N	2.51	0.42
2:M:177:MET:HE2	2:M:327:ALA:CB	2.48	0.42
2:M:199:LYS:HE2	2:M:199:LYS:HA	2.00	0.42
2:O:199:LYS:HE2	2:O:199:LYS:N	2.35	0.42
2:O:339:TYR:CD1	2:O:378:GLU:HG3	2.55	0.42
2:P:497:ASP:CA	2:P:500:VAL:HG12	2.46	0.42
1:B:636:MET:SD	1:B:636:MET:N	2.93	0.42
2:N:151:TRP:C	2:N:153:ILE:N	2.77	0.42
2:N:564:TRP:HZ3	2:N:584:LEU:HD12	1.83	0.42
2:O:363:ASP:OD1	2:O:462:ARG:HA	2.19	0.42
1:A:607:MET:HE1	1:A:634:PHE:CE1	2.55	0.42
1:C:3:ARG:NH1	1:C:625:SER:OG	2.50	0.42
1:C:235:ILE:HG23	1:C:597:SER:OG	2.19	0.42
2:M:339:TYR:CD1	2:M:378:GLU:HG3	2.55	0.42
2:N:376:ILE:HD12	2:N:376:ILE:O	2.19	0.42
1:A:241:ASP:OD2	1:A:245:GLU:OE2	2.37	0.42
1:B:280:LEU:HD13	1:B:288:SER:HB2	2.02	0.42
1:B:559:LEU:HG	1:B:563:MET:HE2	2.00	0.42
1:C:308:LYS:N	1:C:308:LYS:HD2	2.35	0.42
1:D:313:VAL:HB	1:D:331:VAL:CG2	2.41	0.42
1:D:370:ARG:HG2	1:D:370:ARG:HH11	1.84	0.42
2:O:350:PHE:HB3	2:O:478:MET:CE	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.90	0.42
2:P:410:PHE:CE1	2:P:455:GLU:HG3	2.55	0.42
1:D:652:ARG:O	1:D:656:LEU:HB2	2.19	0.42
2:M:376:ILE:HD12	2:M:376:ILE:O	2.19	0.42
2:M:382:LEU:HD12	2:M:383:PRO:HD2	2.01	0.42
2:O:280:GLN:HA	2:O:281:PRO:HD3	1.94	0.42
2:O:282:LEU:HA	2:O:283:PRO:HD3	1.96	0.42
2:O:586:THR:HG22	2:O:588:MET:N	2.33	0.42
2:P:564:TRP:HZ3	2:P:584:LEU:HD12	1.85	0.42
1:B:412:LYS:C	1:B:414:SER:H	2.27	0.41
1:B:445:ALA:HB3	1:C:38:VAL:HG13	2.01	0.41
1:C:370:ARG:HG2	1:C:370:ARG:HH11	1.85	0.41
1:C:409:LYS:O	1:C:413:GLU:HG2	2.20	0.41
1:D:415:ASN:C	1:D:417:PRO:HD3	2.45	0.41
1:D:439:LEU:CD1	1:D:537:ILE:HD13	2.49	0.41
2:N:199:LYS:HE2	2:N:199:LYS:N	2.35	0.41
2:N:496:THR:HB	2:N:523:GLU:OE2	2.20	0.41
2:P:572:TYR:HA	2:P:579:LEU:O	2.20	0.41
2:P:604:ILE:C	2:P:604:ILE:CD1	2.93	0.41
2:P:604:ILE:CD1	2:P:606:PRO:HD3	2.50	0.41
1:A:238:ALA:O	1:A:241:ASP:HB3	2.20	0.41
1:A:469:GLY:O	1:A:500:CYS:HB2	2.20	0.41
1:C:412:LYS:HD3	1:C:416:ARG:HE	1.85	0.41
2:M:556:GLU:OE2	2:M:559:PRO:HB3	2.20	0.41
2:N:399:PHE:O	2:N:403:LEU:HD13	2.19	0.41
2:O:346:ARG:HG3	2:O:346:ARG:NH1	2.36	0.41
2:P:162:ARG:HB2	2:P:188:GLU:HB2	2.02	0.41
1:A:52:PHE:CZ	1:A:474:LYS:HA	2.55	0.41
1:B:52:PHE:CZ	1:B:474:LYS:HA	2.55	0.41
1:D:443:GLN:HB2	1:D:451:VAL:HG21	2.02	0.41
1:D:483:THR:HB	1:D:638:PRO:HB2	2.02	0.41
2:N:587:LEU:HD23	2:N:588:MET:CE	2.50	0.41
2:N:597:CYS:HB3	7:N:950:ACT:O	2.20	0.41
2:O:424:ASN:H	2:O:424:ASN:ND2	2.16	0.41
2:O:725:MET:HG2	2:O:726:ASP:OD1	2.20	0.41
1:B:12:ARG:HB3	1:B:13:PRO:HD2	2.02	0.41
1:B:652:ARG:O	1:B:656:LEU:HB2	2.20	0.41
2:M:405:ARG:CZ	8:M:1049:HOH:O	2.67	0.41
2:O:471:GLU:O	2:O:475:LYS:CG	2.68	0.41
2:O:716:GLU:HG2	2:O:723:LEU:HD21	2.02	0.41
1:B:607:MET:HE1	1:B:634:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:THR:HG23	1:C:639:GLN:HE21	1.85	0.41
1:D:394:ILE:HG23	1:D:395:GLU:N	2.34	0.41
2:O:399:PHE:O	2:O:403:LEU:HD13	2.19	0.41
2:O:560:ILE:O	2:O:660:ALA:HB2	2.20	0.41
2:O:572:TYR:HA	2:O:579:LEU:O	2.19	0.41
2:P:199:LYS:HE2	2:P:199:LYS:HA	2.02	0.41
2:P:510:GLN:HA	2:P:513:ALA:O	2.20	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.20	0.41
1:C:303:LYS:HA	1:C:307:ALA:O	2.21	0.41
2:M:61:TYR:O	2:M:63:PRO:HD3	2.21	0.41
2:M:571:LEU:HD21	2:M:579:LEU:HD12	2.01	0.41
2:N:402:VAL:HG13	2:N:535:ASP:OD1	2.20	0.41
2:O:247:ARG:NH2	2:O:514:PRO:HG3	2.36	0.41
1:A:615:LEU:HD13	1:A:615:LEU:C	2.46	0.41
1:B:535:ALA:O	1:B:536:ASN:HB2	2.21	0.41
1:D:483:THR:HG23	1:D:639:GLN:HE21	1.85	0.41
2:M:315:LYS:HD2	8:M:1027:HOH:O	2.21	0.41
2:O:510:GLN:HA	2:O:513:ALA:O	2.20	0.41
2:P:69:SER:OG	2:P:71:GLU:OE1	2.39	0.41
2:P:560:ILE:O	2:P:660:ALA:HB2	2.20	0.41
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.56	0.41
1:C:439:LEU:HD12	1:C:537:ILE:HD13	2.03	0.41
1:C:574:VAL:HA	1:C:575:PRO:HD3	1.91	0.41
1:D:317:CYS:O	1:D:321:GLU:HG2	2.21	0.41
1:D:352:ASP:OD1	1:D:353:VAL:N	2.42	0.41
2:M:86:LYS:HD3	2:M:86:LYS:HA	1.86	0.41
2:N:445:GLY:O	2:N:449:VAL:HG23	2.20	0.41
2:N:700:ALA:CB	2:N:704:ILE:HD11	2.51	0.41
1:A:182:GLU:HB3	1:A:204:VAL:HG11	2.02	0.41
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.86	0.41
1:C:105:MET:HE1	1:C:609:PRO:HD2	2.02	0.41
2:M:282:LEU:HA	2:M:283:PRO:HD3	1.96	0.41
2:M:342:MET:N	2:M:342:MET:SD	2.94	0.41
2:M:564:TRP:HZ3	2:M:584:LEU:HD12	1.86	0.41
2:N:156:GLU:HG3	2:N:182:MET:HB3	2.03	0.41
2:N:655:LYS:HE2	8:N:1272:HOH:O	2.20	0.41
2:O:605:LEU:HD11	2:O:612:MET:HB3	2.03	0.41
2:O:704:ILE:HD13	2:O:714:TYR:CD2	2.55	0.41
2:P:579:LEU:HD21	2:P:640:GLN:HG3	2.03	0.41
2:P:586:THR:HG23	2:P:661:ASP:OD1	2.21	0.41
1:A:469:GLY:O	4:A:800:XCC:S1	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLY:C	1:D:318:THR:HG23	2.45	0.41
2:N:572:TYR:HA	2:N:579:LEU:O	2.21	0.41
2:O:156:GLU:HB2	2:O:250:ALA:HB2	2.03	0.41
2:O:354:ARG:HD2	2:O:389:ASP:OD2	2.21	0.41
2:O:496:THR:O	2:O:500:VAL:HB	2.21	0.41
2:P:313:LEU:HD12	2:P:313:LEU:C	2.46	0.41
1:D:152:ILE:HD12	1:D:166:VAL:CG1	2.51	0.40
2:O:289:PRO:O	2:O:290:ASP:HB2	2.21	0.40
2:P:289:PRO:O	2:P:290:ASP:HB2	2.20	0.40
1:A:218:GLN:HG3	1:B:377:ASN:HB2	2.03	0.40
1:C:483:THR:HB	1:C:638:PRO:HB2	2.02	0.40
1:D:35:GLU:OE1	1:D:419:TYR:OH	2.30	0.40
1:D:600:VAL:HG12	1:D:601:PRO:O	2.21	0.40
2:N:363:ASP:OD1	2:N:462:ARG:HA	2.22	0.40
2:O:373:ILE:HD11	2:O:435:VAL:CG2	2.50	0.40
2:P:423:ARG:HB3	2:P:485:TYR:CE1	2.56	0.40
1:A:267:ASN:O	1:A:270:VAL:HG22	2.21	0.40
1:A:326:GLN:HB2	1:A:328:ILE:HG12	2.03	0.40
1:C:33:VAL:HG12	1:C:37:LEU:CD2	2.51	0.40
1:D:607:MET:HE1	1:D:634:PHE:CE1	2.57	0.40
2:M:424:ASN:H	2:M:424:ASN:ND2	2.15	0.40
2:M:586:THR:HG23	2:M:661:ASP:OD1	2.21	0.40
2:M:723:LEU:CD1	2:M:723:LEU:H	2.35	0.40
2:N:384:LEU:HD11	2:N:467:ILE:HG23	2.04	0.40
2:O:496:THR:H	2:O:499:THR:HB	1.85	0.40
2:P:124:ASP:OD1	2:P:125:GLU:HG3	2.21	0.40
1:A:637:ASP:HA	1:A:638:PRO:HD2	1.95	0.40
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.52	0.40
1:D:305:ALA:CB	1:D:409:LYS:HE3	2.52	0.40
2:M:197:ASN:O	2:M:199:LYS:HE3	2.22	0.40
2:N:9:GLU:OE1	2:N:9:GLU:HA	2.22	0.40
2:N:579:LEU:HD11	2:N:593:THR:HG21	2.02	0.40
2:P:86:LYS:HA	2:P:86:LYS:HD3	1.83	0.40
2:P:587:LEU:HD23	2:P:588:MET:HE1	2.02	0.40
1:A:186:LEU:CD2	1:A:205:PRO:HD2	2.52	0.40
1:C:16:ALA:HB2	8:C:908:HOH:O	2.21	0.40
1:C:157:LYS:NZ	8:C:870:HOH:O	2.54	0.40
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.52	0.40
2:M:323:ASN:HD22	2:M:323:ASN:HA	1.74	0.40
2:M:602:MET:HE1	2:M:645:MET:HE3	2.04	0.40
2:N:199:LYS:HE2	2:N:199:LYS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:500:VAL:O	2:O:553:LYS:NZ	2.54	0.40
2:O:556:GLU:OE2	2:O:559:PRO:HB3	2.21	0.40
2:P:424:ASN:H	2:P:424:ASN:ND2	2.16	0.40

There are no symmetry-related clashes.

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	670/674 (99%)	646 (96%)	21 (3%)	3 (0%)	30	34
1	B	670/674 (99%)	644 (96%)	22 (3%)	4 (1%)	21	23
1	C	670/674 (99%)	647 (97%)	21 (3%)	2 (0%)	36	42
1	D	670/674 (99%)	646 (96%)	22 (3%)	2 (0%)	36	42
2	M	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	21	23
2	N	726/729 (100%)	696 (96%)	26 (4%)	4 (1%)	21	23
2	O	726/729 (100%)	682 (94%)	34 (5%)	10 (1%)	9	7
2	P	726/729 (100%)	691 (95%)	29 (4%)	6 (1%)	16	16
All	All	5584/5612 (100%)	5348 (96%)	201 (4%)	35 (1%)	21	23

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	316	ILE
2	O	315	LYS
1	B	415	ASN
1	A	267	ASN
1	B	267	ASN
2	M	187	ASP
2	M	679	HIS

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Mol	Chain	Res	Type
2	N	187	ASP
2	N	679	HIS
2	O	187	ASP
2	O	317	LYS
2	O	319	ASP
2	O	470	ASP
2	O	679	HIS
2	P	187	ASP
2	P	319	ASP
2	P	679	HIS
1	A	354	GLN
1	B	354	GLN
1	B	413	GLU
1	C	267	ASN
1	C	354	GLN
1	D	267	ASN
1	D	354	GLN
2	M	596	GLY
2	N	596	GLY
2	O	596	GLY
2	P	596	GLY
2	P	727	PRO
1	A	416	ARG
2	O	726	ASP
2	P	295	VAL
2	O	295	VAL
2	O	721	PRO
2	N	295	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	541/543 (100%)	525 (97%)	16 (3%)	36	49
1	B	541/543 (100%)	525 (97%)	16 (3%)	36	49
1	C	541/543 (100%)	527 (97%)	14 (3%)	40	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	541/543 (100%)	526 (97%)	15 (3%)	38	52
2	M	610/611 (100%)	590 (97%)	20 (3%)	33	45
2	N	610/611 (100%)	590 (97%)	20 (3%)	33	45
2	O	610/611 (100%)	591 (97%)	19 (3%)	35	48
2	P	610/611 (100%)	593 (97%)	17 (3%)	38	52
All	All	4604/4616 (100%)	4467 (97%)	137 (3%)	36	49

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	37	LEU
1	A	42	ASP
1	A	148	ARG
1	A	166	VAL
1	A	206	PHE
1	A	217	ASN
1	A	331	VAL
1	A	377	ASN
1	A	415	ASN
1	A	517	GLU
1	A	518	THR
1	A	539	ILE
1	A	615	LEU
1	A	653	THR
1	A	656	LEU
1	B	3	ARG
1	B	37	LEU
1	B	42	ASP
1	B	148	ARG
1	B	166	VAL
1	B	206	PHE
1	B	217	ASN
1	B	331	VAL
1	B	377	ASN
1	B	416	ARG
1	B	517	GLU
1	B	518	THR
1	B	539	ILE
1	B	615	LEU

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Mol	Chain	Res	Type
1	B	653	THR
1	B	656	LEU
1	C	3	ARG
1	C	37	LEU
1	C	42	ASP
1	C	148	ARG
1	C	166	VAL
1	C	206	PHE
1	C	217	ASN
1	C	331	VAL
1	C	377	ASN
1	C	517	GLU
1	C	518	THR
1	C	615	LEU
1	C	653	THR
1	C	656	LEU
1	D	3	ARG
1	D	37	LEU
1	D	42	ASP
1	D	148	ARG
1	D	166	VAL
1	D	206	PHE
1	D	217	ASN
1	D	331	VAL
1	D	377	ASN
1	D	517	GLU
1	D	518	THR
1	D	539	ILE
1	D	615	LEU
1	D	653	THR
1	D	656	LEU
2	M	17	GLU
2	M	21	LEU
2	M	66	ARG
2	M	71	GLU
2	M	174	LYS
2	M	199	LYS
2	M	209	LEU
2	M	214	GLN
2	M	216	VAL
2	M	238	GLU
2	M	317	LYS

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Mol	Chain	Res	Type
2	M	318	LEU
2	M	342	MET
2	M	406	ARG
2	M	424	ASN
2	M	428	LEU
2	M	553	LYS
2	M	571	LEU
2	M	702	GLU
2	M	704	ILE
2	N	9	GLU
2	N	21	LEU
2	N	66	ARG
2	N	71	GLU
2	N	174	LYS
2	N	199	LYS
2	N	209	LEU
2	N	214	GLN
2	N	216	VAL
2	N	315	LYS
2	N	342	MET
2	N	406	ARG
2	N	424	ASN
2	N	428	LEU
2	N	553	LYS
2	N	571	LEU
2	N	604	ILE
2	N	702	GLU
2	N	704	ILE
2	N	723	LEU
2	O	14	GLU
2	O	21	LEU
2	O	66	ARG
2	O	71	GLU
2	O	174	LYS
2	O	199	LYS
2	O	209	LEU
2	O	214	GLN
2	O	216	VAL
2	O	318	LEU
2	O	342	MET
2	O	406	ARG
2	O	424	ASN

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Mol	Chain	Res	Type
2	O	428	LEU
2	O	482	ARG
2	O	553	LYS
2	O	571	LEU
2	O	702	GLU
2	O	704	ILE
2	P	21	LEU
2	P	66	ARG
2	P	71	GLU
2	P	174	LYS
2	P	199	LYS
2	P	209	LEU
2	P	214	GLN
2	P	216	VAL
2	P	318	LEU
2	P	342	MET
2	P	406	ARG
2	P	424	ASN
2	P	428	LEU
2	P	553	LYS
2	P	571	LEU
2	P	702	GLU
2	P	704	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	56	GLN
1	A	58	GLN
1	A	164	GLN
1	A	217	ASN
1	A	225	ASN
1	A	275	GLN
1	A	293	GLN
1	A	377	ASN
1	A	415	ASN
1	A	471	ASN
1	A	639	GLN
1	B	9	HIS
1	B	56	GLN
1	B	58	GLN

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Mol	Chain	Res	Type
1	B	164	GLN
1	B	217	ASN
1	B	225	ASN
1	B	275	GLN
1	B	377	ASN
1	B	446	GLN
1	B	454	GLN
1	B	471	ASN
1	B	639	GLN
1	C	9	HIS
1	C	56	GLN
1	C	58	GLN
1	C	122	HIS
1	C	164	GLN
1	C	217	ASN
1	C	225	ASN
1	C	275	GLN
1	C	377	ASN
1	C	415	ASN
1	C	454	GLN
1	C	471	ASN
1	C	536	ASN
1	C	639	GLN
1	D	9	HIS
1	D	56	GLN
1	D	58	GLN
1	D	118	ASN
1	D	122	HIS
1	D	164	GLN
1	D	217	ASN
1	D	225	ASN
1	D	275	GLN
1	D	377	ASN
1	D	454	GLN
1	D	471	ASN
1	D	565	ASN
1	D	639	GLN
2	M	211	ASN
2	M	214	GLN
2	M	240	GLN
2	M	287	GLN
2	M	323	ASN

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Mol	Chain	Res	Type
2	M	375	GLN
2	M	422	GLN
2	M	424	ASN
2	M	516	HIS
2	N	211	ASN
2	N	214	GLN
2	N	240	GLN
2	N	287	GLN
2	N	323	ASN
2	N	375	GLN
2	N	422	GLN
2	N	424	ASN
2	N	515	ASN
2	N	516	HIS
2	N	576	ASN
2	N	581	GLN
2	N	590	ASN
2	O	211	ASN
2	O	214	GLN
2	O	240	GLN
2	O	287	GLN
2	O	323	ASN
2	O	375	GLN
2	O	422	GLN
2	O	424	ASN
2	O	515	ASN
2	O	516	HIS
2	O	576	ASN
2	O	618	HIS
2	P	27	HIS
2	P	211	ASN
2	P	214	GLN
2	P	240	GLN
2	P	287	GLN
2	P	323	ASN
2	P	375	GLN
2	P	422	GLN
2	P	424	ASN
2	P	515	ASN
2	P	516	HIS
2	P	576	ASN

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 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	$\# Z > 2$
4	XCC	B	800	1	0,12,12	-	-	-		
3	SF4	A	700	1	0,12,12	-	-	-		
4	XCC	C	800	1	0,12,12	-	-	-		
3	SF4	M	900	2	0,12,12	-	-	-		
7	ACT	P	950	5	1,2,3	1.92	0	0,1,3	-	-
3	SF4	D	750	1	0,12,12	-	-	-		
3	SF4	P	900	2	0,12,12	-	-	-		
4	XCC	A	800	1	0,12,12	-	-	-		
7	ACT	O	950	5	1,2,3	1.76	0	0,1,3	-	-
7	ACT	M	950	-	1,2,3	1.82	0	0,1,3	-	-
3	SF4	B	750	1	0,12,12	-	-	-		
4	XCC	D	800	1	0,12,12	-	-	-		
3	SF4	C	750	1	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	C	700	1	0,12,12	-	-	-		
7	ACT	N	950	-	1,2,3	2.22	1 (100%)	0,1,3	-	-
3	SF4	N	900	2	0,12,12	-	-	-		
3	SF4	O	900	2	0,12,12	-	-	-		

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
4	XCC	B	800	1	-	-	0/4/4/4
3	SF4	A	700	1	-	-	0/6/5/5
4	XCC	C	800	1	-	-	0/4/4/4
3	SF4	M	900	2	-	-	0/6/5/5
3	SF4	D	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
4	XCC	A	800	1	-	-	0/4/4/4
3	SF4	B	750	1	-	-	0/6/5/5
4	XCC	D	800	1	-	-	0/4/4/4
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
3	SF4	N	900	2	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	N	950	ACT	O-C	2.22	1.29	1.20

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	XCC	2	0
4	C	800	XCC	3	0
7	P	950	ACT	1	0
4	A	800	XCC	3	0
7	O	950	ACT	1	0
7	M	950	ACT	2	0
4	D	800	XCC	2	0
7	N	950	ACT	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

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.