



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 05:03 pm BST

PDB ID : 3I01  
Title : Native structure of bifunctional carbon monoxide dehydrogenase/acetyl-CoA synthase from Moorella thermoacetica, water-bound C-cluster.  
Authors : Kung, Y.; Doukov, T.I.; Drennan, C.L.  
Deposited on : 2009-06-24  
Resolution : 2.15 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

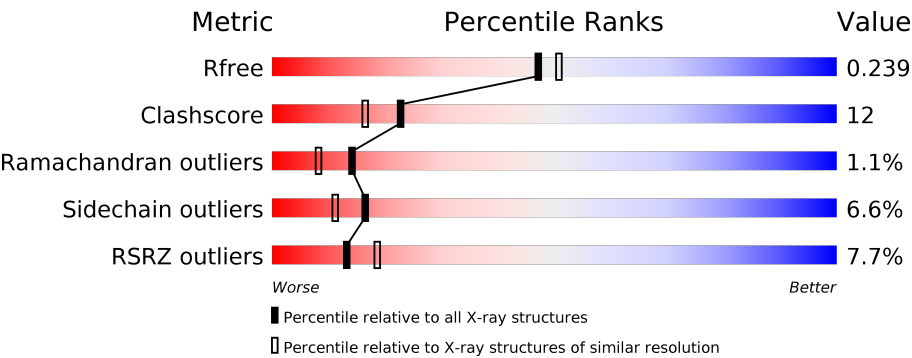
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	674	
1	B	674	
1	C	674	
1	D	674	
2	M	729	
2	N	729	

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Mol	Chain	Length	Quality of chain
2	O	729	
2	P	729	

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
3	SF4	O	900	-	-	X	-
4	XCC	D	800	-	-	X	-
5	GOL	C	863	-	-	X	-
5	GOL	D	863	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45096 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.

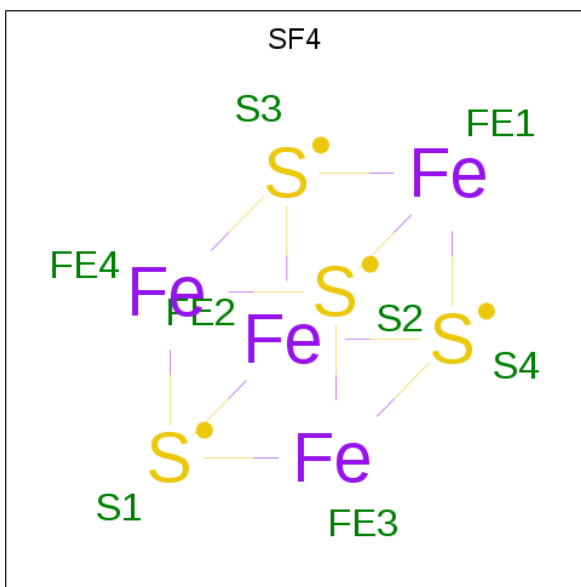
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	7	0
			5128	3223	897	966	42			
1	B	673	Total	C	N	O	S	0	5	0
			5121	3221	895	963	42			
1	C	673	Total	C	N	O	S	0	2	0
			5094	3205	888	959	42			
1	D	673	Total	C	N	O	S	0	4	0
			5119	3218	895	964	42			

- Molecule 2 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha.

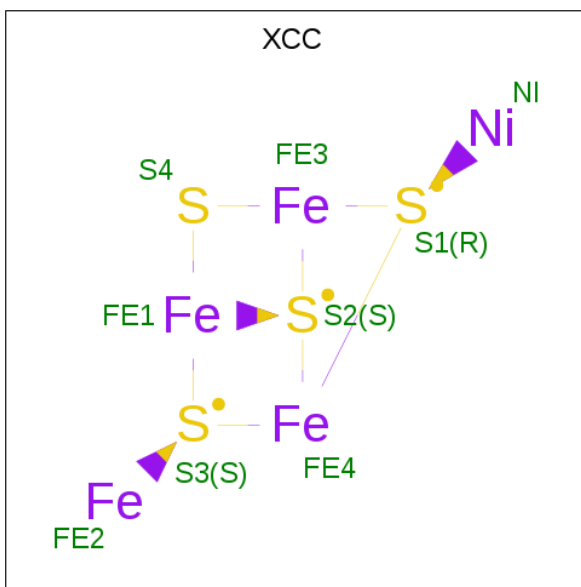
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	5	0
			5778	3703	964	1076	35			
2	N	728	Total	C	N	O	S	0	6	0
			5784	3707	968	1074	35			
2	O	728	Total	C	N	O	S	0	1	0
			5749	3687	958	1069	35			
2	P	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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 (three-letter code: XCC) (formula: Fe<sub>4</sub>NiS<sub>4</sub>).



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 GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 7 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	P	1	Total	Na	0	0
			1	1		
9	O	1	Total	Na	0	0
			1	1		
9	N	1	Total	Na	0	0
			1	1		
9	M	1	Total	Na	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	215	Total	O	0	0
			215	215		

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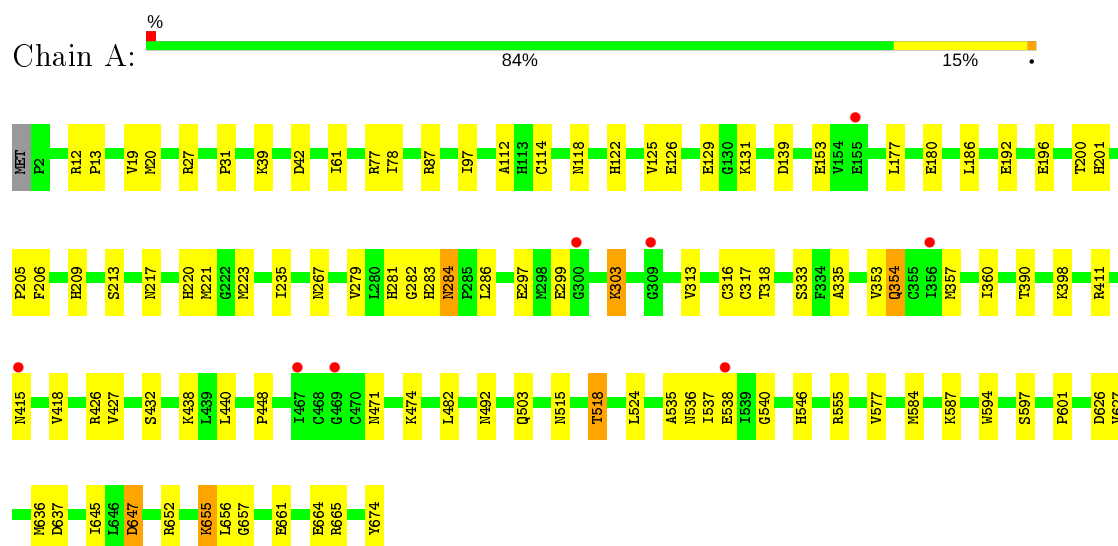
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	288	Total 288	O 288	0	0
10	C	169	Total 169	O 169	0	0
10	D	151	Total 151	O 151	0	0
10	M	218	Total 218	O 218	0	0
10	N	227	Total 227	O 227	0	0
10	O	27	Total 27	O 27	0	0
10	P	118	Total 118	O 118	0	0

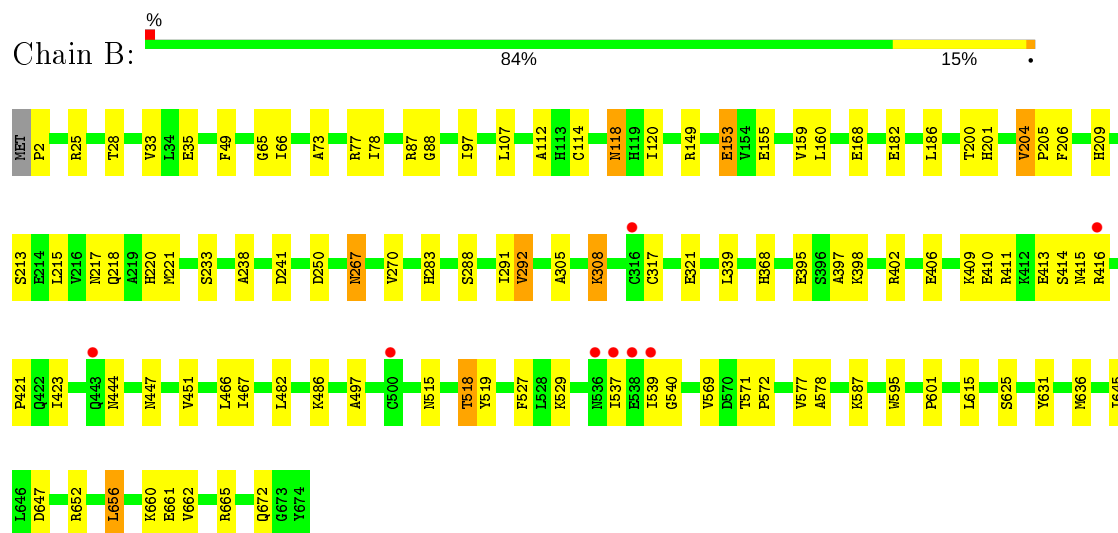
### 3 Residue-property plots [i](#)

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

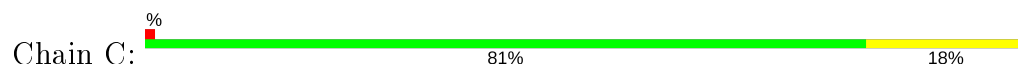
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

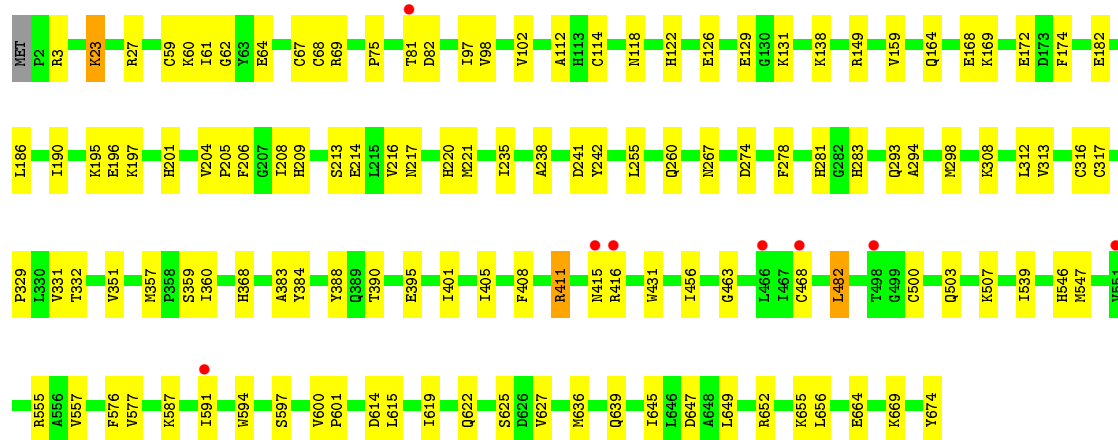


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

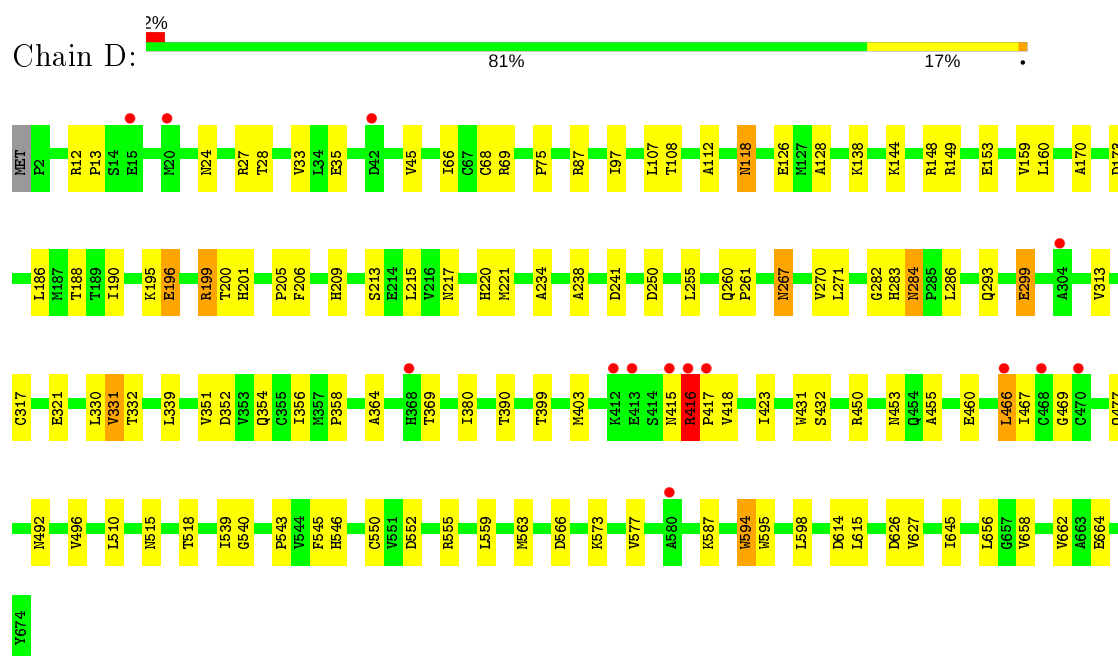


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

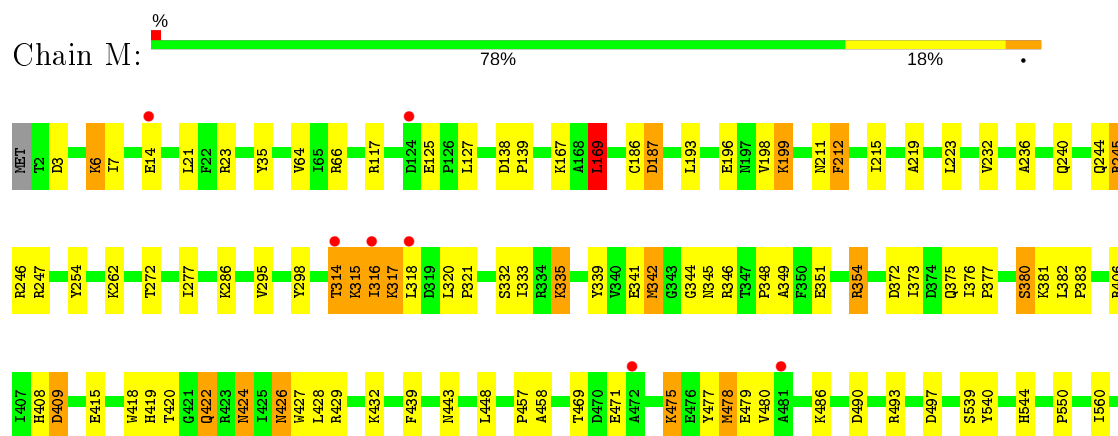


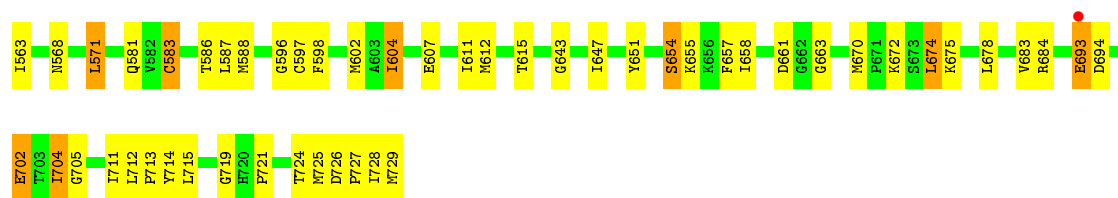


• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

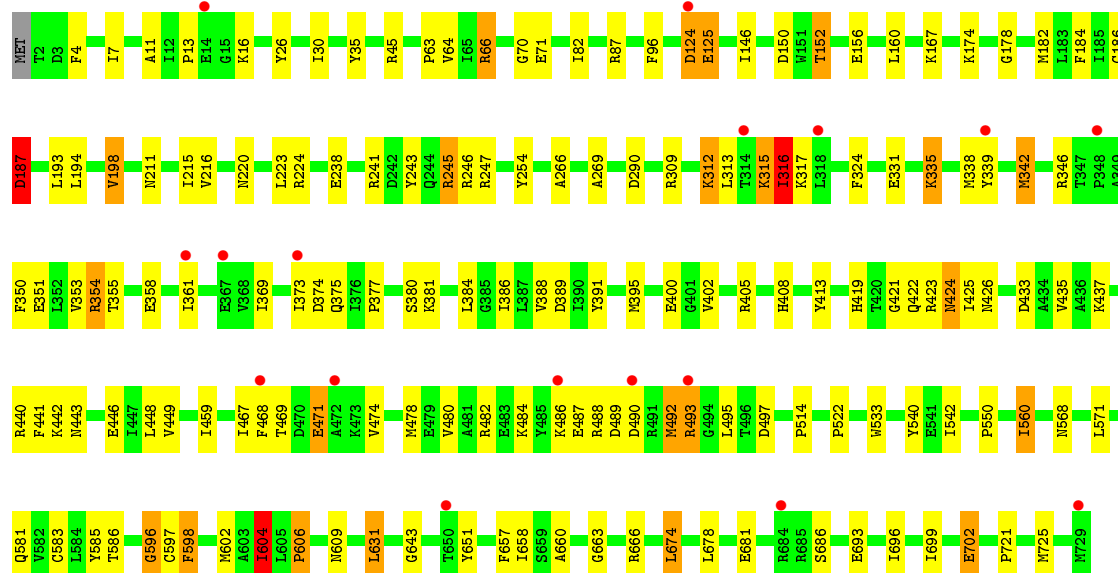
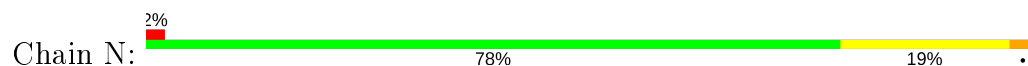


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

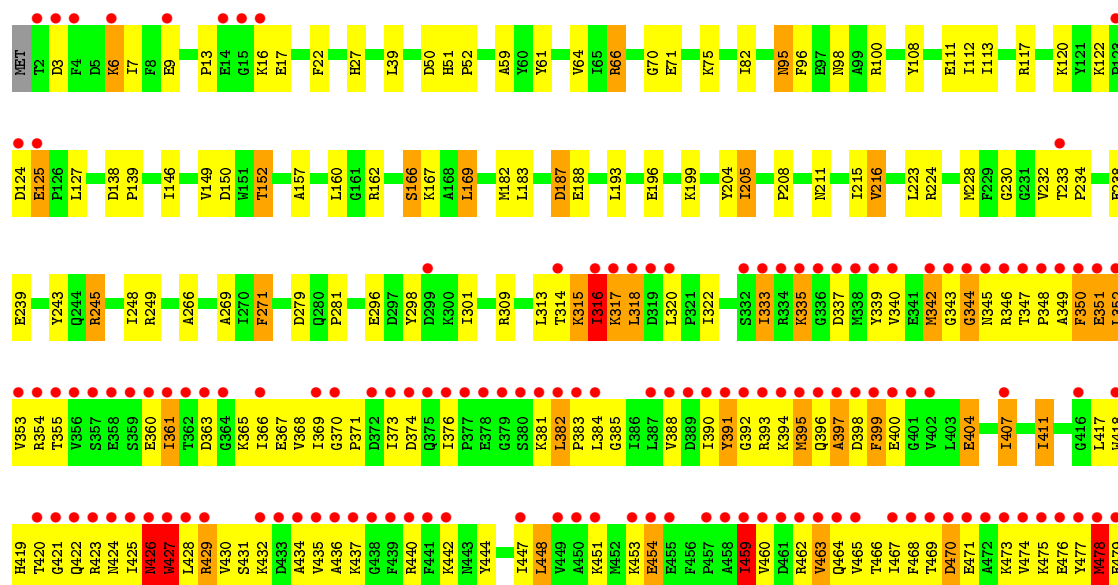
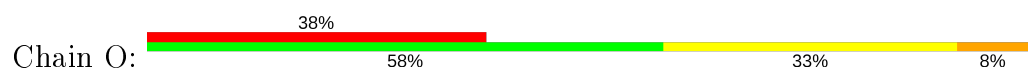


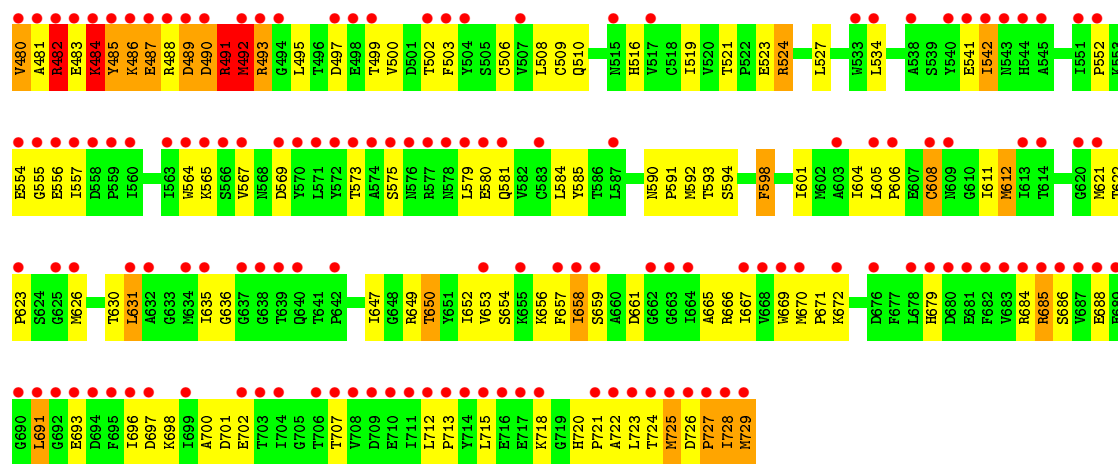


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

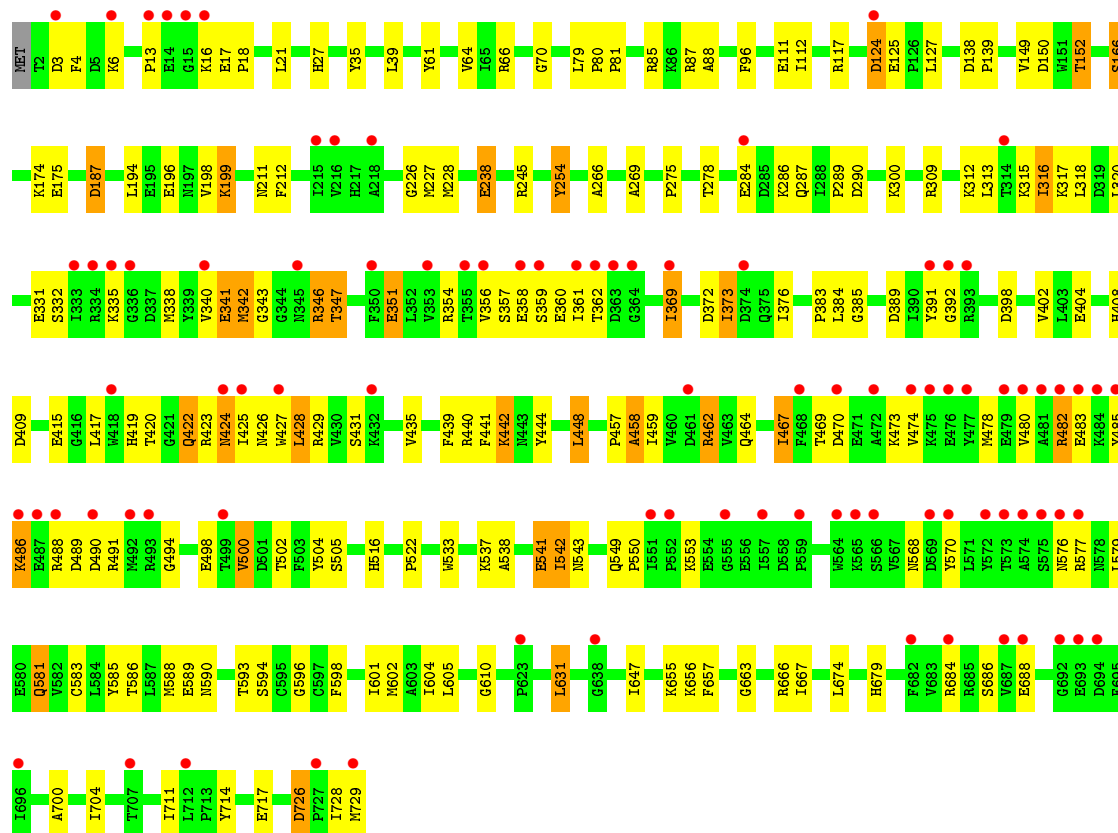
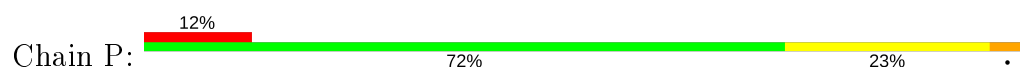


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha





• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.65Å 136.87Å 140.86Å 101.26° 109.11° 104.08°	Depositor
Resolution (Å)	36.96 – 2.15 36.54 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.96-2.15) 92.3 (36.54-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.186 , 0.242 0.187 , 0.239	Depositor DCC
$R_{free}$ test set	16243 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	45096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CU1, NI, NA, SF4, ACT, XCC

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	1.06	0/5244	0.91	6/7106 (0.1%)
1	B	1.11	6/5231 (0.1%)	0.92	3/7086 (0.0%)
1	C	1.06	6/5193 (0.1%)	0.90	2/7038 (0.0%)
1	D	0.95	1/5212 (0.0%)	0.90	3/7062 (0.0%)
2	M	1.00	5/5921 (0.1%)	0.89	7/8015 (0.1%)
2	N	0.99	3/5928 (0.1%)	0.91	8/8023 (0.1%)
2	O	0.89	1/5883 (0.0%)	0.89	7/7965 (0.1%)
2	P	0.86	0/5885	0.83	2/7968 (0.0%)
All	All	0.99	22/44497 (0.0%)	0.89	38/60263 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	388	TYR	CD1-CE1	5.96	1.48	1.39
2	O	725	MET	C-O	-5.83	1.12	1.23
1	B	292	VAL	CB-CG1	5.82	1.65	1.52
2	N	184	PHE	CE2-CZ	5.80	1.48	1.37
2	M	186	CYS	CB-SG	5.76	1.92	1.82
2	N	186	CYS	CB-SG	5.75	1.92	1.82
1	C	242	TYR	CD2-CE2	5.54	1.47	1.39
1	C	415	ASN	N-CA	-5.54	1.35	1.46
1	C	415	ASN	C-O	-5.47	1.12	1.23
1	B	527	PHE	CE1-CZ	5.41	1.47	1.37
2	M	298	TYR	CD1-CE1	5.37	1.47	1.39
1	D	196	GLU	CB-CG	5.28	1.62	1.52
1	B	204	VAL	CB-CG1	5.22	1.63	1.52
1	B	168	GLU	CG-CD	5.22	1.59	1.51
2	M	232	VAL	CB-CG1	5.21	1.63	1.52
1	C	411	ARG	CZ-NH2	5.21	1.39	1.33
1	C	500	CYS	CB-SG	-5.21	1.73	1.81
1	B	321	GLU	CG-CD	5.18	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	583	CYS	CB-SG	-5.15	1.73	1.81
2	M	212	PHE	CE2-CZ	5.12	1.47	1.37
1	B	578	ALA	CA-CB	-5.02	1.42	1.52
2	N	216	VAL	CB-CG2	-5.01	1.42	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	597	CYS	CA-CB-SG	-5.99	103.21	114.00
2	O	685	ARG	N-CA-CB	-5.98	99.83	110.60
2	M	597	CYS	CA-CB-SG	-5.93	103.32	114.00
1	B	339	LEU	CA-CB-CG	-5.89	101.75	115.30
1	B	87	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	O	344	GLY	N-CA-C	5.76	127.50	113.10
1	A	87	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	O	491	ARG	N-CA-C	-5.70	95.62	111.00
2	N	241	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	N	702	GLU	CB-CA-C	-5.62	99.16	110.40
1	D	87	ARG	NE-CZ-NH1	-5.55	117.53	120.30
2	N	631	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	555	ARG	NE-CZ-NH2	-5.51	117.54	120.30
2	N	187	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	87	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	411	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	N	87	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	O	426	ASN	CB-CA-C	-5.44	99.51	110.40
2	O	427	TRP	N-CA-CB	-5.42	100.83	110.60
2	P	85	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	M	497	ASP	CB-CG-OD1	5.34	123.11	118.30
2	M	169	LEU	CB-CG-CD2	5.31	120.02	111.00
1	D	416	ARG	N-CA-C	5.31	125.33	111.00
1	C	3	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	594	TRP	CA-CB-CG	5.28	123.73	113.70
2	M	571	LEU	CA-CB-CG	5.27	127.41	115.30
2	M	678	LEU	CA-CB-CG	5.26	127.39	115.30
2	M	661	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	647	ASP	CB-CG-OD2	-5.18	113.64	118.30
2	O	490	ASP	N-CA-C	5.17	124.95	111.00
2	O	478	MET	N-CA-C	5.14	124.89	111.00
2	M	661	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	637	ASP	CB-CG-OD2	5.11	122.90	118.30
2	P	227	MET	CG-SD-CE	5.10	108.37	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ASP	CB-CG-OD2	5.04	122.83	118.30
2	N	224	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	N	604	ILE	CB-CA-C	-5.01	101.57	111.60
1	D	550	CYS	CA-CB-SG	-5.01	104.98	114.00

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	5128	0	5128	62	0
1	B	5121	0	5134	71	0
1	C	5094	0	5097	89	0
1	D	5119	0	5115	99	0
2	M	5778	0	5736	96	0
2	N	5784	0	5749	106	0
2	O	5749	0	5716	377	0
2	P	5746	0	5710	142	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	1	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	1	0
3	O	8	0	0	2	0
3	P	8	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	2	0
5	A	6	0	8	0	0
5	B	6	0	7	0	0
5	C	6	0	8	5	0
5	D	6	0	8	6	0
6	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	M	3	0	3	0	0
8	N	3	0	3	0	0
8	O	3	0	3	1	0
8	P	3	0	3	1	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
10	A	215	0	0	5	0
10	B	288	0	0	4	0
10	C	169	0	0	6	0
10	D	151	0	0	3	0
10	M	218	0	0	5	0
10	N	227	0	0	6	0
10	O	27	0	0	2	0
10	P	118	0	0	6	0
All	All	45096	0	43428	1002	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 12.

All (1002) 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)
2:O:482:ARG:CZ	2:O:482:ARG:HA	1.72	1.19
2:O:490:ASP:HB2	2:O:491:ARG:NH1	1.61	1.16
2:O:685:ARG:O	2:O:688:GLU:HB3	1.44	1.15
2:O:482:ARG:NH1	2:O:482:ARG:HA	1.62	1.13
2:M:335:LYS:H	2:M:335:LYS:HD2	1.07	1.12
2:O:477:TYR:O	2:O:480:VAL:HB	1.51	1.10
2:N:335:LYS:H	2:N:335:LYS:CD	1.66	1.09
2:O:490:ASP:HB2	2:O:491:ARG:HH12	1.09	1.08
2:N:335:LYS:HD3	2:N:335:LYS:N	1.65	1.08
2:M:602:MET:CE	2:M:647:ILE:HD13	1.84	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.19	1.07
2:P:588:MET:CE	2:P:604:ILE:HD13	1.88	1.04
2:O:420:THR:OG1	2:O:427:TRP:HE3	1.38	1.04
2:O:487:GLU:HG2	2:O:488:ARG:N	1.67	1.04
2:O:557:ILE:HD11	2:O:565:LYS:HG3	1.35	1.03
2:N:246[B]:ARG:HH12	2:N:247:ARG:NH1	1.56	1.02
2:P:444:TYR:O	2:P:448:LEU:HD22	1.60	1.02
2:O:371:PRO:HD2	2:O:469:THR:OG1	1.56	1.01
2:N:315:LYS:HE2	2:N:315:LYS:H	1.22	1.01
2:O:604:ILE:HD12	2:O:606:PRO:HD3	1.41	1.00
2:O:483:GLU:O	2:O:486:LYS:HB3	1.59	1.00
2:N:335:LYS:HD3	2:N:335:LYS:H	0.83	1.00
2:O:351:GLU:HG2	2:O:423:ARG:H	1.27	0.99
2:O:483:GLU:CG	2:O:484:LYS:H	1.77	0.97
2:O:427:TRP:C	2:O:428:LEU:HD22	1.85	0.96
2:O:483:GLU:HG3	2:O:484:LYS:N	1.77	0.96
2:O:487:GLU:HG2	2:O:488:ARG:H	1.26	0.96
2:O:343:GLY:CA	2:O:349:ALA:HB2	1.95	0.96
2:O:348:PRO:CB	2:O:475:LYS:HE2	1.94	0.95
2:O:487:GLU:CG	2:O:488:ARG:N	2.30	0.95
2:O:348:PRO:HB3	2:O:475:LYS:HE2	1.48	0.95
2:O:482:ARG:CA	2:O:482:ARG:CZ	2.44	0.95
2:O:391:TYR:CD2	2:O:462:ARG:HB2	2.00	0.95
2:O:466:THR:C	2:O:467:ILE:HD12	1.86	0.95
2:O:723:LEU:HD23	2:O:723:LEU:C	1.86	0.94
2:O:418:TRP:CH2	2:O:420:THR:HG21	2.02	0.94
2:O:348:PRO:CG	2:O:475:LYS:HE2	1.97	0.94
2:O:418:TRP:CH2	2:O:420:THR:CG2	2.51	0.93
1:D:539:ILE:HG23	1:D:540:GLY:N	1.84	0.92
2:N:484:LYS:HG2	10:N:1375:HOH:O	1.68	0.92
2:O:418:TRP:CZ3	2:O:420:THR:HG23	2.05	0.92
2:O:351:GLU:HB2	2:O:426:ASN:ND2	1.85	0.92
2:M:335:LYS:N	2:M:335:LYS:HD2	1.86	0.91
2:P:13:PRO:HB2	2:P:16:LYS:HG3	1.53	0.91
2:O:367:GLU:OE2	2:O:369:ILE:HD11	1.69	0.90
2:O:483:GLU:CG	2:O:484:LYS:N	2.30	0.90
2:P:602:MET:CE	2:P:647:ILE:HG21	2.02	0.90
2:P:588:MET:HE1	2:P:604:ILE:HD13	1.50	0.90
2:M:602:MET:HE1	2:M:647:ILE:HD13	1.55	0.89
2:M:602:MET:HE3	2:M:647:ILE:HD13	1.53	0.88
2:M:341:GLU:OE1	2:M:381:LYS:HE3	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:480:VAL:O	2:O:483:GLU:HG2	1.74	0.87
2:N:315:LYS:N	2:N:315:LYS:HE2	1.90	0.87
2:O:376:ILE:HG21	2:O:382:LEU:HD21	1.56	0.86
2:O:351:GLU:HB3	2:O:423:ARG:N	1.89	0.86
2:O:351:GLU:CG	2:O:423:ARG:H	1.88	0.86
1:D:416:ARG:O	1:D:418:VAL:HG23	1.76	0.86
2:M:335:LYS:H	2:M:335:LYS:CD	1.88	0.86
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.05	0.85
2:O:715:LEU:HD22	2:O:720:HIS:HD2	1.40	0.85
2:P:470:ASP:HA	10:P:1362:HOH:O	1.75	0.85
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.56	0.85
2:O:653:VAL:O	2:O:685:ARG:HD2	1.77	0.84
2:O:370:GLY:HA3	2:O:469:THR:OG1	1.79	0.83
2:P:588:MET:HE3	2:P:604:ILE:HD13	1.59	0.83
2:O:685:ARG:NH1	2:O:685:ARG:HB3	1.93	0.83
2:O:350:PHE:CD2	2:O:385:GLY:HA3	2.14	0.82
2:O:365:LYS:HG2	2:O:464:GLN:HG3	1.60	0.82
2:O:418:TRP:CZ3	2:O:420:THR:CG2	2.62	0.82
2:P:4:PHE:HB2	2:P:238:GLU:OE2	1.79	0.82
5:D:863:GOL:H2	2:P:27:HIS:HE1	1.43	0.82
2:O:723:LEU:HD23	2:O:723:LEU:O	1.79	0.82
2:O:396:GLN:HG3	2:O:399:PHE:CD1	2.15	0.81
2:P:150:ASP:OD2	2:P:152:THR:HG22	1.79	0.81
5:C:863:GOL:H31	2:O:27:HIS:CE1	2.15	0.81
2:O:419:HIS:HE1	2:O:421:GLY:O	1.64	0.80
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.61	0.80
2:M:704:ILE:HD11	2:M:711:ILE:HA	1.61	0.80
1:C:577[A]:VAL:HG21	1:C:645:ILE:HG23	1.62	0.80
1:D:539:ILE:CG2	1:D:540:GLY:N	2.44	0.80
2:O:348:PRO:CG	2:O:475:LYS:CE	2.59	0.80
2:O:490:ASP:CB	2:O:491:ARG:NH1	2.42	0.80
2:O:666:ARG:NH2	2:O:725:MET:HE2	1.96	0.80
2:O:350:PHE:HD2	2:O:385:GLY:HA3	1.42	0.80
2:O:351:GLU:CB	2:O:426:ASN:HD21	1.95	0.80
1:C:220:HIS:HD2	1:C:221:MET:O	1.65	0.79
2:O:343:GLY:HA2	2:O:349:ALA:HB2	1.65	0.79
2:O:421:GLY:HA3	2:O:425:ILE:O	1.82	0.79
1:A:535:ALA:HB3	1:A:537:ILE:CD1	2.12	0.79
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.19	0.78
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.65	0.78
2:M:587:LEU:HD23	2:M:588:MET:HE1	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:490:ASP:O	2:N:493:ARG:HG3	1.84	0.78
2:O:467:ILE:N	2:O:467:ILE:HD12	1.98	0.78
2:O:351:GLU:HG2	2:O:423:ARG:N	1.99	0.78
2:O:351:GLU:HB2	2:O:426:ASN:HD21	1.46	0.78
2:O:381:LYS:O	2:O:383:PRO:HD3	1.84	0.77
1:B:529:LYS:CB	10:B:1156:HOH:O	2.32	0.77
2:M:320:LEU:HB3	2:M:321:PRO:HD2	1.66	0.77
2:M:471:GLU:O	2:M:475:LYS:HB2	1.83	0.77
2:P:361:ILE:HG13	2:P:464:GLN:HG2	1.67	0.77
2:O:396:GLN:NE2	2:O:399:PHE:CD1	2.51	0.77
2:O:480:VAL:HA	2:O:483:GLU:OE1	1.84	0.77
5:C:863:GOL:H31	2:O:27:HIS:HE1	1.46	0.77
2:M:7:ILE:HD13	2:M:245:ARG:HD2	1.64	0.77
2:M:426:ASN:HD22	2:M:426:ASN:H	1.32	0.77
2:O:363:ASP:OD1	2:O:462:ARG:HA	1.85	0.77
1:B:529:LYS:HB3	10:B:1156:HOH:O	1.85	0.76
1:D:577[A]:VAL:HG21	1:D:645:ILE:HG23	1.67	0.76
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.21	0.76
2:N:346:ARG:HB3	2:N:381:LYS:HD2	1.66	0.76
2:O:649:ARG:HA	2:O:652:ILE:HD12	1.66	0.76
2:O:483:GLU:HG2	2:O:484:LYS:H	1.48	0.76
1:C:614:ASP:H	5:C:863:GOL:H32	1.51	0.76
1:B:35:GLU:OE1	1:B:421:PRO:HB3	1.86	0.75
2:P:424:ASN:H	2:P:424:ASN:HD22	1.32	0.75
1:A:284:ASN:HD22	1:A:286:LEU:H	1.34	0.75
5:D:863:GOL:H2	2:P:27:HIS:CE1	2.21	0.75
2:N:478:MET:O	2:N:482:ARG:HG3	1.85	0.75
2:P:150:ASP:OD2	2:P:152:THR:CG2	2.35	0.75
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.52	0.75
2:O:478:MET:O	2:O:481:ALA:HB3	1.88	0.74
2:O:384:LEU:HD12	2:O:385:GLY:H	1.52	0.74
2:O:464:GLN:NE2	2:O:466:THR:HG23	2.02	0.73
1:C:209:HIS:HD2	1:D:213:SER:CB	2.02	0.73
1:C:60:LYS:O	1:C:64:GLU:HG3	1.87	0.73
2:O:371:PRO:CD	2:O:469:THR:OG1	2.34	0.73
2:O:351:GLU:O	2:O:352:LEU:HB3	1.88	0.73
2:O:374:ASP:HB3	2:O:440:ARG:NE	2.03	0.73
2:P:316:ILE:HG23	2:P:316:ILE:O	1.88	0.73
1:A:577[B]:VAL:HG11	1:A:645:ILE:HG23	1.69	0.72
2:M:406:ARG:NH1	2:M:409:ASP:OD2	2.20	0.72
1:A:192:GLU:O	1:A:196:GLU:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:480:VAL:HG12	2:O:481:ALA:N	2.02	0.72
2:O:353:VAL:HG12	2:O:388:VAL:HB	1.72	0.72
1:D:510:LEU:N	1:D:510:LEU:HD12	2.05	0.72
2:O:491:ARG:H	2:O:491:ARG:NH1	1.88	0.71
2:O:723:LEU:CD2	2:O:723:LEU:C	2.59	0.71
2:O:349:ALA:HB3	2:O:424:ASN:O	1.91	0.71
2:O:351:GLU:HB3	2:O:423:ARG:CA	2.20	0.71
2:O:347:THR:HG23	2:O:383:PRO:HG3	1.72	0.71
2:O:626:MET:HB2	2:O:631:LEU:HD13	1.73	0.71
2:O:355:THR:OG1	2:O:395:MET:HG3	1.91	0.70
2:O:650:THR:HG22	2:O:650:THR:O	1.91	0.70
1:D:299:GLU:OE2	1:D:299:GLU:HA	1.91	0.70
2:O:157:ALA:HB3	2:O:183:LEU:HD22	1.71	0.70
2:O:349:ALA:HB1	2:O:426:ASN:OD1	1.91	0.70
2:O:557:ILE:CD1	2:O:565:LYS:HG3	2.17	0.70
2:O:666:ARG:NH2	2:O:725:MET:CE	2.54	0.70
2:P:505:SER:HB3	2:P:570:TYR:CE2	2.26	0.70
2:O:343:GLY:HA3	2:O:349:ALA:HB2	1.72	0.70
2:O:396:GLN:HG3	2:O:399:PHE:HD1	1.56	0.70
2:O:476:GLU:C	2:O:476:GLU:OE1	2.30	0.70
2:P:359:SER:C	2:P:361:ILE:H	1.93	0.69
2:O:509:CYS:HB3	8:O:953:ACT:H3	1.74	0.69
2:O:396:GLN:C	2:O:396:GLN:OE1	2.30	0.69
2:O:666:ARG:CZ	2:O:725:MET:CE	2.71	0.69
2:O:478:MET:O	2:O:481:ALA:N	2.25	0.69
2:O:484:LYS:O	2:O:485:TYR:C	2.30	0.69
2:N:384:LEU:HD11	2:N:467:ILE:CG2	2.22	0.69
2:O:396:GLN:HE22	2:O:398:ASP:HB2	1.57	0.69
2:O:374:ASP:HB3	2:O:440:ARG:HE	1.58	0.69
2:O:427:TRP:O	2:O:428:LEU:HD22	1.93	0.69
2:O:728:ILE:O	2:O:728:ILE:HD12	1.92	0.68
2:O:108:TYR:O	2:O:112:ILE:HG13	1.93	0.68
2:O:524:ARG:O	2:O:524:ARG:HG3	1.93	0.68
1:C:601:PRO:HD3	1:C:652:ARG:NH2	2.09	0.68
2:O:685:ARG:O	2:O:688:GLU:CB	2.33	0.68
2:P:486:LYS:HA	2:P:489:ASP:HB2	1.76	0.67
2:O:333:ILE:HD12	2:O:429:ARG:HB3	1.76	0.67
2:P:149:VAL:HG11	8:P:953:ACT:H3	1.76	0.67
2:N:408:HIS:HD2	2:N:419:HIS:ND1	1.91	0.67
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.75	0.67
2:O:486:LYS:O	2:O:489:ASP:HB3	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:614:ASP:N	5:D:863:GOL:H11	2.09	0.67
2:M:439:PHE:CE1	2:M:443:ASN:HB2	2.29	0.67
2:O:162:ARG:HG3	2:O:188:GLU:HB2	1.77	0.67
2:M:377:PRO:O	2:M:380:SER:HB3	1.94	0.67
2:O:348:PRO:HG2	2:O:475:LYS:CE	2.25	0.67
2:O:605:LEU:HB3	2:O:608:CYS:HB2	1.77	0.67
1:D:68:CYS:HB2	1:D:97:ILE:CG2	2.24	0.67
2:O:360:GLU:O	2:O:361:ILE:HB	1.94	0.67
2:O:365:LYS:HG2	2:O:464:GLN:CG	2.24	0.66
2:M:23:ARG:NH1	10:M:793:HOH:O	2.27	0.66
2:P:80:PRO:HB2	2:P:81:PRO:HD3	1.76	0.66
1:C:209:HIS:HD2	1:D:213:SER:OG	1.78	0.66
2:M:424:ASN:H	2:M:424:ASN:HD22	1.43	0.66
2:P:444:TYR:O	2:P:448:LEU:CD2	2.39	0.66
2:O:691:LEU:HD21	2:O:721:PRO:HG2	1.76	0.66
2:O:340:VAL:HG21	2:O:382:LEU:HB2	1.78	0.66
2:O:351:GLU:CB	2:O:426:ASN:ND2	2.56	0.66
1:D:149[A]:ARG:HD3	10:D:1162:HOH:O	1.96	0.65
1:C:213:SER:CB	1:D:209:HIS:HD2	2.08	0.65
1:D:284:ASN:HD22	1:D:286:LEU:H	1.42	0.65
2:M:426:ASN:HD22	2:M:426:ASN:N	1.94	0.65
2:O:230:GLY:HA3	2:O:243:TYR:CE2	2.32	0.65
2:O:342:MET:O	2:O:427:TRP:HA	1.95	0.65
2:O:469:THR:O	2:O:470:ASP:HB2	1.95	0.65
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.09	0.65
2:O:224:ARG:O	2:O:228:MET:HB2	1.95	0.65
2:O:715:LEU:HD22	2:O:720:HIS:CD2	2.29	0.65
2:O:384:LEU:C	2:O:474:VAL:HG21	2.17	0.65
2:O:3:ASP:O	2:O:6:LYS:HG2	1.97	0.65
2:O:422:GLN:N	2:O:422:GLN:OE1	2.30	0.65
2:O:384:LEU:HD13	2:O:468:PHE:O	1.97	0.65
2:O:685:ARG:HH11	2:O:685:ARG:HB3	1.62	0.65
1:C:98:VAL:O	1:C:102:VAL:HG12	1.97	0.64
1:C:260:GLN:HG2	10:C:1398:HOH:O	1.97	0.64
2:O:407:ILE:HG23	2:O:411:ILE:HD13	1.77	0.64
2:O:428:LEU:N	2:O:428:LEU:HD22	2.12	0.64
2:O:124:ASP:C	2:O:125:GLU:HG2	2.18	0.64
2:O:480:VAL:O	2:O:481:ALA:C	2.34	0.64
2:M:655:LYS:HE3	10:M:901:HOH:O	1.96	0.64
2:O:469:THR:O	2:O:470:ASP:CB	2.45	0.64
1:D:515:ASN:HA	1:D:518:THR:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:602:MET:HE3	2:P:647:ILE:HG21	1.80	0.64
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.32	0.64
1:D:195:LYS:O	1:D:199:ARG:HG3	1.97	0.64
2:N:335:LYS:N	2:N:335:LYS:CD	2.40	0.64
1:C:587:LYS:O	1:C:591:ILE:HG13	1.98	0.64
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.28	0.64
2:N:246[B]:ARG:HH12	2:N:247:ARG:HH11	1.43	0.64
2:N:443:ASN:ND2	2:N:446:GLU:OE1	2.30	0.64
2:M:721:PRO:O	2:M:725:MET:HG3	1.97	0.64
1:C:615:LEU:HD23	1:C:615:LEU:C	2.18	0.64
2:O:473:LYS:C	2:O:476:GLU:H	2.02	0.63
2:O:352:LEU:CD1	2:O:484:LYS:HG3	2.28	0.63
2:O:508:LEU:HD23	3:O:900:SF4:S1	2.38	0.63
2:N:150:ASP:OD2	2:N:152:THR:HG22	1.99	0.63
2:O:482:ARG:CA	2:O:482:ARG:NE	2.59	0.63
2:M:344:GLY:O	2:M:346:ARG:NH1	2.32	0.63
2:O:447:ILE:O	2:O:451:LYS:HB2	1.98	0.63
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.34	0.63
2:N:492:MET:HG2	10:N:1002:HOH:O	1.97	0.63
2:N:540:TYR:CD1	2:N:550:PRO:HD3	2.34	0.63
2:N:609:ASN:ND2	2:N:666:ARG:HH12	1.97	0.62
2:O:169:LEU:HD13	2:O:193:LEU:CD2	2.29	0.62
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.34	0.62
1:C:294:ALA:O	1:C:298:MET:HG2	1.99	0.62
1:C:587:LYS:H	1:D:220:HIS:HE1	1.48	0.62
2:M:568:ASN:HD21	2:M:581:GLN:HE21	1.48	0.62
1:C:615:LEU:HD23	1:C:615:LEU:O	2.00	0.62
2:N:315:LYS:N	2:N:315:LYS:CE	2.63	0.62
2:O:64:VAL:HB	2:O:223:LEU:HD12	1.81	0.62
1:C:23:LYS:HE3	10:C:931:HOH:O	1.98	0.61
2:O:404:GLU:OE1	2:O:423:ARG:NE	2.34	0.61
2:O:564:TRP:HB2	2:O:567:VAL:HB	1.82	0.61
2:P:666:ARG:HD2	2:P:728:ILE:HD12	1.81	0.61
2:N:354:ARG:HD2	2:N:389:ASP:OD2	2.00	0.61
1:B:200:THR:OG1	1:B:201:HIS:HD2	1.84	0.61
2:O:490:ASP:O	2:O:492:MET:N	2.33	0.61
2:P:583:CYS:CB	2:P:586:THR:HG22	2.30	0.61
1:A:114:CYS:HB2	10:A:1315:HOH:O	2.00	0.61
2:O:95:ASN:ND2	2:O:98:ASN:H	1.98	0.61
2:M:348:PRO:HD2	2:M:383:PRO:HB3	1.82	0.61
2:P:316:ILE:CG2	2:P:316:ILE:O	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:66:ARG:O	2:P:70:GLY:HA2	2.01	0.61
1:C:220:HIS:HE1	1:D:587:LYS:H	1.49	0.61
2:M:704:ILE:HD13	2:M:714:TYR:CB	2.30	0.61
2:O:420:THR:O	2:O:426:ASN:HA	2.00	0.61
2:O:385:GLY:N	2:O:474:VAL:HG21	2.16	0.61
2:P:341:GLU:CD	2:P:427:TRP:HE1	2.04	0.61
2:P:289:PRO:O	2:P:290:ASP:HB2	2.00	0.61
1:A:122:HIS:HD2	10:A:902:HOH:O	1.83	0.61
2:O:478:MET:O	2:O:482:ARG:N	2.33	0.61
2:P:166:SER:HB2	2:P:196:GLU:OE2	1.99	0.61
2:P:359:SER:O	2:P:361:ILE:N	2.34	0.61
2:M:342:MET:N	2:M:342:MET:SD	2.73	0.61
2:O:360:GLU:O	2:O:361:ILE:CB	2.49	0.61
2:O:351:GLU:CB	2:O:423:ARG:N	2.62	0.60
1:B:515:ASN:HA	1:B:518:THR:HG23	1.84	0.60
2:O:420:THR:HG1	2:O:427:TRP:HE3	0.65	0.60
2:M:457:PRO:O	2:M:458:ALA:HB3	2.00	0.60
2:O:346:ARG:HH22	2:O:381:LYS:NZ	2.00	0.60
2:P:726:ASP:OD1	2:P:726:ASP:N	2.33	0.60
2:O:557:ILE:HD11	2:O:565:LYS:CG	2.22	0.60
2:P:602:MET:HG3	2:P:647:ILE:HD13	1.83	0.60
1:A:220:HIS:HD2	1:A:221:MET:O	1.84	0.60
1:A:655:LYS:NZ	1:A:674:TYR:O	2.28	0.60
2:O:351:GLU:CB	2:O:423:ARG:H	2.15	0.60
1:D:399:THR:O	1:D:403:MET:HG3	2.02	0.60
2:O:388:VAL:HG13	2:O:465:VAL:HG22	1.84	0.60
2:P:428:LEU:HD12	2:P:428:LEU:N	2.16	0.60
2:O:426:ASN:N	2:O:426:ASN:OD1	2.34	0.59
2:P:199:LYS:HE2	2:P:415:GLU:OE2	2.03	0.59
2:N:560:ILE:O	2:N:660:ALA:HB2	2.02	0.59
2:M:167:LYS:HD3	2:M:196:GLU:OE1	2.01	0.59
2:O:347:THR:CG2	2:O:383:PRO:HG3	2.32	0.59
2:O:712:LEU:HB3	2:O:713:PRO:CD	2.31	0.59
1:D:510:LEU:HD12	1:D:510:LEU:H	1.65	0.59
2:M:314:THR:O	2:M:315:LYS:C	2.39	0.59
1:A:535:ALA:HB3	1:A:537:ILE:HD12	1.85	0.59
2:P:238:GLU:HG2	10:P:735:HOH:O	2.01	0.59
2:O:169:LEU:HD13	2:O:193:LEU:HD21	1.85	0.59
1:A:284:ASN:HD21	1:A:286:LEU:HG	1.68	0.59
1:D:149[A]:ARG:NH2	1:D:250:ASP:OD2	2.36	0.59
2:P:340:VAL:HG21	2:P:376:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:384:LEU:HD11	2:N:467:ILE:HG23	1.85	0.58
2:O:467:ILE:N	2:O:467:ILE:CD1	2.65	0.58
2:O:666:ARG:CZ	2:O:725:MET:HE1	2.33	0.58
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.34	0.58
2:O:470:ASP:O	2:O:474:VAL:HG12	2.02	0.58
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.85	0.58
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.68	0.58
1:A:316:CYS:H	1:A:503:GLN:HE22	1.52	0.58
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.69	0.58
2:N:150:ASP:OD2	2:N:152:THR:CG2	2.52	0.58
2:P:457:PRO:O	2:P:458:ALA:HB2	2.03	0.58
1:C:456:ILE:HD13	1:C:463:GLY:HA2	1.86	0.58
1:B:661[A]:GLU:HG3	1:B:665:ARG:HH21	1.66	0.58
2:O:367:GLU:OE1	2:O:369:ILE:HG12	2.04	0.58
2:O:665:ALA:O	2:O:722:ALA:HB2	2.03	0.58
1:A:220:HIS:HE1	1:B:587:LYS:H	1.52	0.57
1:D:466:LEU:HD22	1:D:595:TRP:HZ2	1.66	0.57
2:O:355:THR:HG21	2:O:395:MET:HB3	1.86	0.57
2:O:396:GLN:OE1	2:O:397:ALA:N	2.37	0.57
1:C:577[B]:VAL:HG23	1:C:649:LEU:CD2	2.35	0.57
1:D:577[A]:VAL:HG21	1:D:645:ILE:CG2	2.34	0.57
2:P:318:LEU:HD13	2:P:320:LEU:HD11	1.85	0.57
1:C:368:HIS:HE1	1:C:416:ARG:CB	2.18	0.57
2:O:384:LEU:CD1	2:O:468:PHE:O	2.53	0.57
2:O:464:GLN:HE22	2:O:466:THR:HG23	1.67	0.57
2:O:6:LYS:O	2:O:9:GLU:HB2	2.04	0.57
2:P:568:ASN:ND2	2:P:581:GLN:HB2	2.19	0.57
2:M:602:MET:HE3	2:M:647:ILE:CD1	2.29	0.57
2:N:315:LYS:CA	2:N:315:LYS:CE	2.78	0.57
2:N:316:ILE:O	2:N:317:LYS:C	2.42	0.57
2:O:685:ARG:CZ	2:O:685:ARG:HB3	2.31	0.57
1:C:138:LYS:HG3	1:C:255:LEU:O	2.05	0.57
1:B:267:ASN:O	1:B:270:VAL:HG22	2.05	0.56
2:M:727:PRO:HG3	2:O:367:GLU:HG2	1.86	0.56
2:O:477:TYR:O	2:O:480:VAL:CB	2.41	0.56
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.87	0.56
1:D:128:ALA:HA	1:D:160:LEU:HD22	1.87	0.56
2:O:157:ALA:HB3	2:O:183:LEU:HD23	1.87	0.56
1:B:368:HIS:NE2	1:B:416:ARG:HD2	2.20	0.56
2:O:232:VAL:CG1	2:O:239:GLU:HB3	2.35	0.56
2:O:623:PRO:HA	2:O:707:THR:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:357:MET:O	1:C:360:ILE:HG12	2.05	0.56
2:O:340:VAL:HG23	2:O:382:LEU:H	1.70	0.56
1:B:577[A]:VAL:HG21	1:B:645:ILE:HG23	1.88	0.56
1:B:2:PRO:N	1:B:625:SER:HG	2.03	0.56
2:N:246[B]:ARG:NH1	2:N:247:ARG:NH1	2.41	0.56
2:N:369:ILE:HD12	2:N:468:PHE:CE2	2.41	0.56
2:O:483:GLU:HG3	2:O:484:LYS:H	1.44	0.56
1:A:335:ALA:H	1:A:471:ASN:HD22	1.52	0.56
2:O:248:ILE:O	2:O:309:ARG:NH2	2.37	0.56
1:A:126:GLU:OE1	1:A:390:THR:OG1	2.21	0.55
2:O:370:GLY:HA3	2:O:469:THR:HG1	1.71	0.55
2:O:649:ARG:HA	2:O:652:ILE:CD1	2.34	0.55
1:D:149[B]:ARG:NH2	1:D:250:ASP:OD2	2.38	0.55
2:N:315:LYS:CA	2:N:315:LYS:HE2	2.36	0.55
2:P:588:MET:HE3	2:P:604:ILE:CD1	2.35	0.55
1:C:213:SER:OG	1:D:209:HIS:HD2	1.89	0.55
1:D:220:HIS:HD2	1:D:221:MET:O	1.88	0.55
2:M:354:ARG:HH21	2:M:480:VAL:HG11	1.71	0.55
2:M:408:HIS:HD2	2:M:419:HIS:ND1	2.05	0.55
2:N:342:MET:SD	2:N:342:MET:N	2.79	0.55
2:O:333:ILE:HD12	2:O:429:ARG:CB	2.36	0.55
2:O:473:LYS:O	2:O:476:GLU:HB3	2.07	0.55
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.88	0.55
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.71	0.55
2:N:482:ARG:O	2:N:486[A]:LYS:HG3	2.05	0.55
1:D:144:LYS:O	1:D:148:ARG:HG3	2.06	0.55
2:O:340:VAL:CG2	2:O:382:LEU:H	2.19	0.55
2:O:430:VAL:HG12	2:O:431:SER:N	2.21	0.55
2:P:424:ASN:ND2	2:P:424:ASN:H	2.01	0.55
2:O:396:GLN:CG	2:O:399:PHE:CD1	2.90	0.55
1:C:614:ASP:H	5:C:863:GOL:C3	2.18	0.54
2:N:442:LYS:HB2	10:N:1326:HOH:O	2.06	0.54
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.90	0.54
2:N:721:PRO:O	2:N:725:MET:HG3	2.07	0.54
2:O:721:PRO:O	2:O:725:MET:HB2	2.07	0.54
2:P:424:ASN:N	2:P:424:ASN:HD22	1.99	0.54
1:B:539:ILE:HG13	1:B:540:GLY:H	1.72	0.54
1:A:213:SER:OG	1:B:209:HIS:HD2	1.90	0.54
1:B:35:GLU:OE2	1:B:423:ILE:HD11	2.07	0.54
2:P:522:PRO:HD3	2:P:533:TRP:CD1	2.43	0.54
2:M:117[B]:ARG:CZ	2:M:127:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:720:HIS:ND1	2:O:721:PRO:HD2	2.22	0.54
1:C:129:GLU:OE2	1:C:164:GLN:NE2	2.40	0.54
2:O:500:VAL:HG22	2:O:502:THR:H	1.73	0.54
2:P:383:PRO:HB2	2:P:474:VAL:HG21	1.90	0.54
1:C:182:GLU:HG2	1:C:204:VAL:HG11	1.88	0.54
2:O:342:MET:SD	2:O:428:LEU:HB2	2.48	0.54
2:O:396:GLN:CG	2:O:399:PHE:HD1	2.21	0.54
2:O:95:ASN:HD22	2:O:95:ASN:C	2.11	0.54
2:M:490:ASP:HA	2:M:493:ARG:NH1	2.23	0.53
2:P:488:ARG:C	2:P:490:ASP:H	2.12	0.53
1:B:28:THR:HG21	1:B:33:VAL:HG12	1.91	0.53
1:C:408:PHE:O	1:C:411:ARG:HB3	2.07	0.53
1:D:313:VAL:HG21	1:D:331:VAL:HG13	1.90	0.53
1:B:201:HIS:HE1	2:N:35:TYR:OH	1.91	0.53
1:B:444:ASN:HB3	1:B:451:VAL:HG23	1.91	0.53
1:B:529:LYS:HB2	10:B:1156:HOH:O	2.01	0.53
1:C:214:GLU:O	1:C:217:ASN:HB3	2.08	0.53
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.74	0.53
1:B:615:LEU:HD23	1:B:615:LEU:C	2.29	0.53
2:O:351:GLU:HB3	2:O:426:ASN:HD21	1.70	0.53
2:P:359:SER:C	2:P:361:ILE:N	2.61	0.53
1:A:201:HIS:CE1	2:M:35:TYR:OH	2.61	0.53
1:B:656:LEU:HD22	1:B:660:LYS:HD2	1.89	0.53
2:O:478:MET:O	2:O:481:ALA:CB	2.54	0.53
1:D:614:ASP:H	5:D:863:GOL:H11	1.72	0.53
2:N:400:GLU:HB3	2:N:488:ARG:NH2	2.24	0.53
2:O:424:ASN:ND2	2:O:485:TYR:CE1	2.76	0.53
2:M:478:MET:O	2:M:478:MET:HG3	2.09	0.53
2:P:602:MET:HE3	2:P:647:ILE:CG2	2.38	0.53
1:B:220:HIS:HD2	1:B:221:MET:O	1.92	0.52
1:C:577[B]:VAL:HG23	1:C:649:LEU:HD23	1.90	0.52
2:O:483:GLU:O	2:O:486:LYS:CB	2.47	0.52
2:P:408:HIS:HD2	2:P:419:HIS:ND1	2.07	0.52
1:A:177:LEU:HB2	1:A:180:GLU:CD	2.29	0.52
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.39	0.52
1:D:587:LYS:HE3	4:D:800:XCC:S4	2.49	0.52
1:A:209:HIS:HD2	1:B:213:SER:OG	1.92	0.52
2:O:351:GLU:HB3	2:O:423:ARG:HA	1.91	0.52
1:A:535:ALA:CB	1:A:537:ILE:CD1	2.87	0.52
2:O:316:ILE:HG13	2:O:454:GLU:HG3	1.92	0.52
2:O:612:MET:HB3	2:O:669:TRP:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:583:CYS:HB2	2:P:586:THR:HG22	1.92	0.52
2:N:583:CYS:HB2	2:N:586:THR:HG22	1.90	0.52
1:D:24:ASN:O	1:D:27:ARG:HG2	2.08	0.52
2:O:488:ARG:HG3	2:O:488:ARG:NH1	2.24	0.52
2:M:272:THR:HG22	2:M:272:THR:O	2.10	0.52
2:O:367:GLU:OE2	2:O:369:ILE:CD1	2.53	0.52
2:O:467:ILE:HG22	2:O:468:PHE:N	2.25	0.52
2:P:369:ILE:HD13	2:P:473:LYS:HD2	1.92	0.52
2:P:505:SER:HB3	2:P:570:TYR:HE2	1.74	0.52
1:D:238:ALA:O	1:D:241:ASP:HB3	2.10	0.51
1:D:469:GLY:C	4:D:800:XCC:S1	2.88	0.51
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.91	0.51
2:O:367:GLU:HB3	2:O:466:THR:HG22	1.91	0.51
2:O:506:CYS:HB3	3:O:900:SF4:S4	2.51	0.51
2:P:583:CYS:SG	2:P:589:GLU:HG2	2.51	0.51
2:M:426:ASN:H	2:M:426:ASN:ND2	2.05	0.51
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.23	0.51
2:O:346:ARG:HH22	2:O:381:LYS:HZ3	1.58	0.51
2:O:698:LYS:HG2	2:O:718:LYS:HD2	1.92	0.51
2:P:583:CYS:HB3	2:P:586:THR:HG22	1.92	0.51
2:M:351:GLU:OE2	2:M:422:GLN:HA	2.11	0.51
2:O:66:ARG:NH1	2:O:234:PRO:HG2	2.25	0.51
2:P:425:ILE:HG22	2:P:425:ILE:O	2.10	0.51
1:D:364:ALA:HB1	1:D:369:THR:HB	1.92	0.51
2:P:150:ASP:CG	2:P:152:THR:HG22	2.30	0.51
2:O:166:SER:HB2	2:O:196:GLU:CG	2.41	0.51
2:O:626:MET:SD	2:O:631:LEU:HD12	2.51	0.51
2:O:684:ARG:NH1	2:O:685:ARG:HG2	2.25	0.51
2:P:422:GLN:HE21	2:P:422:GLN:N	2.08	0.51
2:P:585:TYR:CE2	2:P:656:LYS:HD2	2.45	0.51
1:C:281:HIS:HB3	1:C:351:VAL:HG12	1.92	0.51
2:N:266:ALA:O	2:N:269:ALA:HB3	2.09	0.51
1:D:284:ASN:ND2	1:D:286:LEU:H	2.08	0.51
2:M:670:MET:HE3	2:M:675:LYS:HG3	1.92	0.51
2:N:596:GLY:HA2	2:N:598:PHE:CE2	2.45	0.51
2:O:113:ILE:O	2:O:117:ARG:HG3	2.10	0.51
2:O:473:LYS:O	2:O:476:GLU:CB	2.58	0.51
2:P:684:ARG:O	2:P:688:GLU:HG3	2.11	0.51
1:C:209:HIS:CD2	1:D:213:SER:CB	2.89	0.51
2:M:372:ASP:H	2:M:375:GLN:NE2	2.09	0.51
2:O:384:LEU:HD12	2:O:385:GLY:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:482:ARG:CZ	2:O:482:ARG:N	2.74	0.51
2:O:484:LYS:O	2:O:485:TYR:O	2.29	0.51
2:O:490:ASP:CB	2:O:491:ARG:HH11	2.24	0.51
2:P:358:GLU:HG3	2:P:391:TYR:CE2	2.46	0.51
2:O:160:LEU:HD13	2:O:215:ILE:HD13	1.93	0.50
2:O:365:LYS:CG	2:O:464:GLN:HG3	2.35	0.50
2:O:685:ARG:C	2:O:688:GLU:HB3	2.27	0.50
2:N:7:ILE:HD13	2:N:245:ARG:HD2	1.94	0.50
2:N:419:HIS:HE1	2:N:421:GLY:O	1.94	0.50
2:O:478:MET:C	2:O:480:VAL:N	2.62	0.50
1:A:284:ASN:ND2	1:A:286:LEU:HG	2.26	0.50
2:O:473:LYS:HA	2:O:476:GLU:HB2	1.94	0.50
1:C:577[A]:VAL:HG13	1:C:649:LEU:HD23	1.92	0.50
2:O:398:ASP:C	2:O:400:GLU:H	2.15	0.50
2:O:489:ASP:O	2:O:489:ASP:OD1	2.30	0.50
1:B:569:VAL:HA	1:B:672:GLN:HE22	1.77	0.50
2:N:13:PRO:HB2	2:N:16:LYS:HG3	1.93	0.50
2:O:417:LEU:HD22	2:O:444:TYR:HE1	1.76	0.50
2:O:316:ILE:CG1	2:O:454:GLU:HG3	2.41	0.50
2:O:66:ARG:O	2:O:70:GLY:HA2	2.12	0.50
2:P:266:ALA:O	2:P:269:ALA:HB3	2.11	0.50
2:P:516:HIS:HE1	2:P:593:THR:O	1.94	0.50
1:C:577[A]:VAL:HG13	1:C:649:LEU:CD2	2.41	0.50
2:N:243:TYR:CZ	2:N:247:ARG:HD3	2.46	0.50
2:O:17:GLU:OE1	2:O:22:PHE:HE2	1.95	0.50
1:D:662:VAL:HG21	2:P:194:LEU:HD13	1.93	0.50
2:M:219:ALA:O	2:M:223:LEU:HG	2.12	0.50
2:N:568:ASN:ND2	2:N:581:GLN:HE21	2.09	0.50
2:O:481:ALA:O	2:O:485:TYR:HB2	2.12	0.50
2:O:421:GLY:C	2:O:422:GLN:OE1	2.50	0.50
2:N:124:ASP:OD1	2:N:125:GLU:OE1	2.30	0.49
2:O:344:GLY:O	2:O:345:ASN:OD1	2.30	0.49
2:O:420:THR:OG1	2:O:427:TRP:CE3	2.30	0.49
1:C:201:HIS:HE1	1:C:627:VAL:HG13	1.77	0.49
1:C:220:HIS:CD2	1:C:221:MET:O	2.55	0.49
1:C:655:LYS:NZ	1:C:674:TYR:O	2.33	0.49
1:D:260:GLN:NE2	10:D:1320:HOH:O	2.43	0.49
2:O:373:ILE:HG12	2:O:435:VAL:HG21	1.94	0.49
2:O:470:ASP:O	2:O:474:VAL:CG1	2.60	0.49
2:P:4:PHE:CB	2:P:238:GLU:OE2	2.57	0.49
1:C:114:CYS:HB2	10:C:1242:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:471:GLU:O	2:N:471:GLU:HG3	2.10	0.49
2:P:657:PHE:CE1	2:P:667:ILE:HD11	2.47	0.49
1:A:333:SER:CB	1:A:503:GLN:HE21	2.25	0.49
2:O:491:ARG:N	2:O:491:ARG:NH1	2.58	0.49
1:D:35:GLU:OE2	1:D:423:ILE:CD1	2.60	0.49
2:M:540:TYR:CD1	2:M:550:PRO:HD3	2.47	0.49
2:O:534:LEU:HD13	10:O:1263:HOH:O	2.13	0.49
1:C:69:ARG:HG2	1:C:75:PRO:HB3	1.94	0.49
1:D:559:LEU:O	1:D:563:MET:HG3	2.12	0.49
2:P:64:VAL:HG13	2:P:111:GLU:OE2	2.12	0.49
2:M:169:LEU:HD13	2:M:193:LEU:CD2	2.42	0.49
2:M:602:MET:CE	2:M:647:ILE:CD1	2.74	0.49
2:N:160:LEU:HD13	2:N:215:ILE:HD13	1.94	0.49
2:P:389:ASP:HB2	2:P:464:GLN:HG3	1.94	0.49
1:A:284:ASN:ND2	1:A:286:LEU:H	2.04	0.49
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.31	0.49
2:O:476:GLU:OE1	2:O:476:GLU:O	2.30	0.49
2:O:481:ALA:O	2:O:482:ARG:C	2.51	0.49
2:N:486[B]:LYS:HG3	2:N:487:GLU:N	2.27	0.49
2:N:489:ASP:O	2:N:493:ARG:HG2	2.13	0.49
2:O:59:ALA:HB2	2:O:630:THR:HA	1.94	0.49
2:N:316:ILE:O	2:N:316:ILE:HG23	2.13	0.49
1:D:201:HIS:HE1	2:P:35:TYR:OH	1.96	0.49
1:B:107:LEU:HD21	1:B:215:LEU:HB3	1.94	0.48
1:C:614:ASP:N	5:C:863:GOL:H32	2.24	0.48
2:O:565:LYS:O	2:O:569:ASP:CG	2.51	0.48
1:B:291:ILE:HD13	1:B:397:ALA:HB1	1.95	0.48
1:D:215:LEU:HD22	1:D:234:ALA:HA	1.95	0.48
2:N:468:PHE:HB2	2:N:474:VAL:HG22	1.95	0.48
2:N:522:PRO:HD3	2:N:533:TRP:CD1	2.49	0.48
2:O:344:GLY:H	2:O:349:ALA:HB2	1.78	0.48
2:O:503:PHE:CZ	2:O:521:THR:HG22	2.48	0.48
2:P:341:GLU:HG3	2:P:429:ARG:HG2	1.95	0.48
2:N:63:PRO:HB2	2:N:220:ASN:HB2	1.95	0.48
2:O:354:ARG:O	2:O:390:ILE:N	2.42	0.48
2:O:468:PHE:CZ	2:O:477:TYR:OH	2.59	0.48
1:D:658:VAL:O	1:D:662:VAL:HG23	2.13	0.48
2:N:424:ASN:HD22	2:N:424:ASN:H	1.61	0.48
2:O:393:ARG:NH1	2:O:394:LYS:HG2	2.29	0.48
2:O:418:TRP:HH2	2:O:420:THR:HG21	1.68	0.48
2:P:150:ASP:OD2	2:P:152:THR:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:343:GLY:HA2	2:P:347:THR:O	2.13	0.48
2:M:320:LEU:HB3	2:M:321:PRO:CD	2.40	0.48
2:O:669:TRP:HA	2:O:700:ALA:O	2.13	0.48
1:B:288:SER:O	1:B:292:VAL:HG23	2.12	0.48
1:D:515:ASN:HA	1:D:518:THR:CG2	2.42	0.48
1:D:539:ILE:CG2	1:D:540:GLY:H	2.27	0.48
2:M:604:ILE:HG13	2:M:643:GLY:O	2.14	0.48
1:B:201:HIS:CE1	2:N:35:TYR:OH	2.67	0.48
2:N:497:ASP:OD2	2:N:585:TYR:OH	2.24	0.48
2:O:428:LEU:CD2	2:O:428:LEU:N	2.76	0.48
1:A:19:VAL:HG22	1:A:474:LYS:HG2	1.96	0.48
1:B:368:HIS:CD2	1:B:416:ARG:HD2	2.48	0.48
1:D:267:ASN:O	1:D:270:VAL:HG22	2.13	0.48
2:P:505:SER:CB	2:P:570:TYR:CE2	2.95	0.48
1:C:316:CYS:H	1:C:503:GLN:HE22	1.62	0.48
2:O:348:PRO:HG3	2:O:475:LYS:CE	2.43	0.48
2:P:338:MET:SD	2:P:341:GLU:HB2	2.54	0.48
2:N:609:ASN:ND2	2:N:666:ARG:NH1	2.61	0.48
2:O:430:VAL:CG1	2:O:434:ALA:HB3	2.43	0.48
1:D:28:THR:OG1	1:D:477:GLN:NE2	2.44	0.47
1:D:282:GLY:HA3	1:D:352:ASP:OD1	2.14	0.47
2:M:64:VAL:HA	2:M:223:LEU:HD12	1.96	0.47
2:N:4:PHE:N	2:N:238[B]:GLU:OE1	2.43	0.47
2:N:312:LYS:NZ	2:N:312:LYS:HB3	2.29	0.47
2:O:344:GLY:N	2:O:349:ALA:HB2	2.29	0.47
2:O:371:PRO:HD2	2:O:469:THR:CB	2.41	0.47
2:O:348:PRO:HG3	2:O:475:LYS:HE2	1.90	0.47
2:P:226:GLY:HA3	10:P:1355:HOH:O	2.13	0.47
2:N:350:PHE:C	2:N:350:PHE:CD1	2.87	0.47
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.45	0.47
2:O:424:ASN:CG	2:O:485:TYR:HE1	2.16	0.47
2:O:490:ASP:O	2:O:493:ARG:N	2.42	0.47
2:O:491:ARG:HB2	2:O:491:ARG:CZ	2.43	0.47
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.28	0.47
1:B:661[A]:GLU:HG3	1:B:665:ARG:NH2	2.30	0.47
2:M:615:THR:HG21	2:M:674:LEU:HG	1.96	0.47
2:O:376:ILE:CG2	2:O:382:LEU:HD21	2.37	0.47
1:B:486:LYS:HE2	1:B:519:TYR:CE2	2.49	0.47
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.44	0.47
2:O:523:GLU:HB3	2:O:654:SER:OG	2.15	0.47
2:P:351:GLU:CG	2:P:426:ASN:HD21	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:167:LYS:HG2	10:N:1288:HOH:O	2.14	0.47
2:O:351:GLU:HB3	2:O:423:ARG:H	1.70	0.47
2:O:604:ILE:HA	2:O:611:ILE:HG22	1.95	0.47
2:O:653:VAL:O	2:O:685:ARG:CD	2.56	0.47
2:N:609:ASN:HD21	2:N:666:ARG:HH12	1.60	0.47
2:O:352:LEU:HD11	2:O:484:LYS:HG3	1.95	0.47
2:O:480:VAL:O	2:O:481:ALA:O	2.32	0.47
1:D:201:HIS:CE1	2:P:35:TYR:OH	2.68	0.47
1:C:59:CYS:HB3	1:D:75:PRO:HG2	1.96	0.47
2:O:342:MET:HG3	2:O:384:LEU:HD23	1.97	0.47
2:O:431:SER:HB3	2:O:434:ALA:HB2	1.97	0.47
2:O:594:SER:O	2:O:636:GLY:HA2	2.14	0.47
1:A:201:HIS:HE1	2:M:35:TYR:OH	1.98	0.47
1:C:331:VAL:HG13	1:C:332:THR:N	2.30	0.47
1:D:510:LEU:N	1:D:510:LEU:CD1	2.77	0.47
2:O:138:ASP:N	2:O:139:PRO:CD	2.78	0.47
2:P:402:VAL:HG21	2:P:538:ALA:HB2	1.94	0.47
2:P:373:ILE:HD12	2:P:441:PHE:CE2	2.50	0.47
1:A:357:MET:O	1:A:360:ILE:HG12	2.14	0.47
1:A:209:HIS:HD2	1:B:213:SER:CB	2.28	0.47
2:O:510:GLN:NE2	2:O:516:HIS:O	2.39	0.47
2:O:650:THR:O	2:O:650:THR:CG2	2.60	0.47
1:C:293:GLN:HG2	10:C:1184:HOH:O	2.14	0.47
2:M:540:TYR:O	2:M:544:HIS:HD2	1.97	0.47
2:P:124:ASP:OD1	2:P:125:GLU:OE1	2.33	0.47
2:P:341:GLU:HG2	2:P:428:LEU:O	2.14	0.47
2:P:346:ARG:HB2	2:P:346:ARG:HH11	1.80	0.47
2:M:670:MET:SD	2:M:674:LEU:HD13	2.55	0.46
2:O:477:TYR:O	2:O:480:VAL:N	2.41	0.46
1:B:182:GLU:HG2	1:B:204:VAL:HG11	1.97	0.46
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.45	0.46
1:D:28:THR:HG21	1:D:33:VAL:CG1	2.44	0.46
2:N:178:GLY:HA3	2:N:317:LYS:HE2	1.97	0.46
1:B:114:CYS:SG	1:B:209:HIS:NE2	2.89	0.46
1:C:62:GLY:HA3	3:C:700:SF4:S4	2.55	0.46
2:M:728:ILE:O	2:M:729:MET:HB2	2.15	0.46
2:P:275:PRO:CD	2:P:309:ARG:HD3	2.45	0.46
1:D:118:ASN:HD22	1:D:118:ASN:C	2.19	0.46
1:D:313:VAL:HG21	1:D:331:VAL:CG1	2.46	0.46
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.14	0.46
2:O:590:ASN:N	2:O:591:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:VAL:HA	2:N:223:LEU:HD12	1.96	0.46
2:O:612:MET:SD	2:O:622:THR:HB	2.56	0.46
2:P:482:ARG:HA	2:P:485:TYR:CD1	2.50	0.46
2:P:700:ALA:HA	2:P:704:ILE:HD13	1.98	0.46
1:B:153:GLU:OE1	1:B:155:GLU:CD	2.54	0.46
1:D:317:CYS:O	1:D:321:GLU:HG2	2.14	0.46
1:D:330:LEU:HD23	10:D:946:HOH:O	2.15	0.46
1:D:415:ASN:OD1	1:D:417:PRO:HD3	2.16	0.46
1:D:594:TRP:CE3	1:D:598:LEU:HD12	2.51	0.46
2:O:13:PRO:HB2	2:O:16:LYS:HB2	1.97	0.46
2:O:61:TYR:HD1	2:O:66:ARG:HD2	1.81	0.46
1:D:432:SER:HA	1:D:555:ARG:HD3	1.98	0.46
2:N:351:GLU:OE2	2:N:422:GLN:HA	2.16	0.46
2:N:568:ASN:HD21	2:N:581:GLN:HE21	1.64	0.46
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.51	0.46
2:M:342:MET:HB3	2:M:382:LEU:O	2.16	0.46
2:M:457:PRO:O	2:M:458:ALA:CB	2.64	0.46
2:M:704:ILE:HG13	2:M:705:GLY:N	2.30	0.46
2:O:266:ALA:O	2:O:269:ALA:HB3	2.15	0.46
2:O:430:VAL:CG1	2:O:431:SER:N	2.79	0.46
2:O:435:VAL:C	2:O:437:LYS:H	2.19	0.46
1:A:61:ILE:HD13	1:A:77:ARG:HD2	1.97	0.46
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.97	0.46
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.31	0.46
2:M:344:GLY:O	2:M:345:ASN:HB2	2.16	0.46
2:O:199:LYS:HD2	2:O:204:TYR:OH	2.16	0.46
2:O:343:GLY:HA2	2:O:349:ALA:CB	2.42	0.46
2:O:427:TRP:NE1	2:O:429:ARG:NH2	2.64	0.46
2:P:138:ASP:N	2:P:139:PRO:CD	2.79	0.46
1:B:305:ALA:HB1	1:B:409:LYS:HE3	1.97	0.46
1:D:138:LYS:HG3	1:D:255:LEU:O	2.16	0.46
2:O:337:ASP:O	2:O:432:LYS:N	2.49	0.46
2:O:385:GLY:N	2:O:474:VAL:CG2	2.78	0.46
2:O:471:GLU:O	2:O:475:LYS:HB2	2.15	0.46
2:O:374:ASP:HB3	2:O:440:ARG:CZ	2.46	0.45
2:P:313:LEU:HD13	2:P:315:LYS:HB2	1.99	0.45
2:O:318:LEU:HD12	2:O:320:LEU:HD21	1.97	0.45
2:O:360:GLU:O	2:O:361:ILE:HG22	2.15	0.45
2:O:516:HIS:HD2	2:O:593:THR:OG1	1.98	0.45
2:P:124:ASP:OD2	2:P:124:ASP:N	2.41	0.45
2:P:420:THR:HG23	2:P:427:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:457:PRO:O	2:P:458:ALA:CB	2.64	0.45
2:P:61:TYR:HD1	2:P:66:ARG:HD2	1.81	0.45
1:C:383:ALA:O	2:P:87:ARG:HD3	2.16	0.45
1:A:126:GLU:HG2	1:A:131:LYS:HB2	1.97	0.45
1:A:299:GLU:O	1:A:303:LYS:HG3	2.15	0.45
2:M:333:ILE:HD12	2:M:418:TRP:HB2	1.98	0.45
2:O:474:VAL:HG13	2:O:475:LYS:N	2.30	0.45
2:O:670:MET:O	2:O:701:ASP:HB3	2.16	0.45
2:P:420:THR:CG2	2:P:427:TRP:HB3	2.46	0.45
2:N:353:VAL:HG22	2:N:388:VAL:HB	1.98	0.45
2:M:587:LEU:HD23	2:M:588:MET:CE	2.42	0.45
2:O:7:ILE:HD13	2:O:245:ARG:HD2	1.99	0.45
1:B:25:ARG:O	1:B:49:PHE:HB3	2.17	0.45
1:C:615:LEU:O	1:C:619:ILE:HG13	2.16	0.45
1:D:496:VAL:HA	1:D:545:PHE:O	2.17	0.45
2:N:433:ASP:OD1	2:N:437:LYS:HE2	2.16	0.45
2:O:100:ARG:HB3	2:O:271:PHE:HB2	1.97	0.45
2:O:727:PRO:O	2:O:729:MET:N	2.50	0.45
1:A:125:VAL:O	1:A:129:GLU:HG3	2.17	0.45
1:C:384:TYR:HE2	2:P:88:ALA:CB	2.29	0.45
2:O:232:VAL:HG11	2:O:239:GLU:HB3	1.97	0.45
2:O:585:TYR:CZ	2:O:656:LYS:HD2	2.52	0.45
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.52	0.45
2:O:50:ASP:HA	2:O:75:LYS:HD2	1.99	0.45
1:A:13:PRO:HB3	1:A:636:MET:HE1	1.99	0.45
2:M:246:ARG:HE	2:M:247:ARG:NH1	2.14	0.45
2:O:350:PHE:O	2:O:385:GLY:HA2	2.16	0.45
2:O:391:TYR:CE2	2:O:462:ARG:HD2	2.52	0.45
1:A:281:HIS:ND1	1:A:282:GLY:N	2.65	0.45
1:A:515:ASN:ND2	1:A:518:THR:HG21	2.32	0.45
2:M:657:PHE:O	2:M:663:GLY:HA2	2.17	0.45
2:N:384:LEU:CD1	2:N:467:ILE:CG2	2.93	0.45
2:N:66:ARG:O	2:N:70:GLY:HA2	2.17	0.45
1:C:238:ALA:O	1:C:241:ASP:HB3	2.17	0.45
1:C:468:CYS:HB2	10:C:693:HOH:O	2.17	0.45
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.99	0.45
2:O:592:MET:HB2	2:O:592:MET:HE3	1.74	0.45
2:P:417:LEU:HD21	2:P:439:PHE:CE1	2.52	0.45
1:D:515:ASN:OD1	1:D:518:THR:HG21	2.17	0.44
2:M:420:THR:HG22	2:M:427:TRP:HB3	1.97	0.44
2:N:247:ARG:NH2	2:N:514:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:478:MET:C	2:O:480:VAL:H	2.18	0.44
2:P:361:ILE:HA	2:P:464:GLN:OE1	2.16	0.44
1:B:406:GLU:O	1:B:410:GLU:HG3	2.17	0.44
1:C:283:HIS:CD2	1:C:317:CYS:CB	2.98	0.44
1:D:261:PRO:HG3	1:D:431:TRP:CZ3	2.53	0.44
2:M:604:ILE:HA	2:M:611:ILE:HG22	1.99	0.44
2:N:342:MET:HG2	2:N:384:LEU:HB2	1.98	0.44
2:O:146:ILE:HG13	2:O:146:ILE:O	2.17	0.44
2:O:370:GLY:CA	2:O:469:THR:OG1	2.58	0.44
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.46	0.44
1:A:201:HIS:HE1	1:A:627:VAL:HG13	1.82	0.44
2:P:357:SER:O	2:P:361:ILE:HG22	2.17	0.44
2:P:426:ASN:O	2:P:427:TRP:HB2	2.16	0.44
1:B:515:ASN:CA	1:B:518:THR:HG23	2.47	0.44
2:M:317:LYS:HE2	10:M:862:HOH:O	2.18	0.44
2:M:712:LEU:HB3	2:M:713:PRO:HD3	1.98	0.44
2:O:657:PHE:CE1	2:O:667:ILE:HD11	2.52	0.44
1:B:238:ALA:O	1:B:241:ASP:HB3	2.18	0.44
2:M:651:TYR:O	2:M:654:SER:HB3	2.18	0.44
2:O:396:GLN:C	2:O:396:GLN:CD	2.76	0.44
2:O:519:ILE:CG2	2:O:584:LEU:HD21	2.48	0.44
1:C:201:HIS:CE1	1:C:627:VAL:HG13	2.53	0.44
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.82	0.44
2:M:427:TRP:C	2:M:428:LEU:HD12	2.38	0.44
2:P:117[B]:ARG:HG2	2:P:127:LEU:HD13	2.00	0.44
1:D:455:ALA:HB1	1:D:460:GLU:HG3	1.98	0.44
2:P:318:LEU:HD13	2:P:320:LEU:CD1	2.47	0.44
1:C:126[A]:GLU:HG2	1:C:131:LYS:HB2	1.98	0.44
1:C:149:ARG:HG2	1:C:149:ARG:HH11	1.83	0.44
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.53	0.44
2:M:560:ILE:O	10:M:1386:HOH:O	2.21	0.44
2:N:490:ASP:HA	2:N:493:ARG:HD2	2.00	0.44
1:B:186:LEU:HD22	1:B:205:PRO:HD2	2.00	0.44
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.48	0.44
2:M:236:ALA:O	2:M:240:GLN:HG2	2.18	0.44
2:O:396:GLN:OE1	2:O:398:ASP:N	2.49	0.44
2:O:724:THR:C	2:O:725:MET:O	2.50	0.44
2:P:385:GLY:O	2:P:467:ILE:HA	2.17	0.44
1:A:39:LYS:O	1:A:42:ASP:HB2	2.17	0.43
2:N:45:ARG:HD2	10:N:1293:HOH:O	2.18	0.43
1:C:213:SER:CB	1:D:209:HIS:CD2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:VAL:HG23	1:D:332:THR:H	1.82	0.43
1:D:358:PRO:HA	1:D:380:ILE:HD13	2.00	0.43
1:D:450:ARG:HG3	1:D:450:ARG:O	2.18	0.43
2:N:11:ALA:O	2:N:13:PRO:HD3	2.18	0.43
2:N:26:TYR:CE2	2:N:30:ILE:HD11	2.52	0.43
2:N:355:THR:HG23	2:N:395:MET:HG2	2.00	0.43
2:O:169:LEU:HD13	2:O:193:LEU:HG	2.01	0.43
2:O:473:LYS:O	2:O:476:GLU:N	2.45	0.43
1:A:657:GLY:O	1:A:661[A]:GLU:HG3	2.18	0.43
2:N:391:TYR:CD2	2:N:391:TYR:C	2.91	0.43
2:O:232:VAL:HG13	2:O:239:GLU:HB3	1.99	0.43
2:O:315:LYS:O	2:O:316:ILE:HB	2.18	0.43
2:O:462:ARG:O	2:O:463:VAL:HG23	2.19	0.43
2:P:358:GLU:O	2:P:462:ARG:NH2	2.51	0.43
2:P:576:ASN:O	2:P:577:ARG:HB2	2.18	0.43
2:P:711:ILE:O	2:P:714:TYR:HB3	2.18	0.43
1:A:492:ASN:HA	1:A:524:LEU:HB2	2.00	0.43
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.99	0.43
1:D:107:LEU:HD21	1:D:215:LEU:HB3	2.00	0.43
1:D:351:VAL:HB	1:D:356:ILE:HD13	2.01	0.43
2:M:3:ASP:O	2:M:6[A]:LYS:HB3	2.18	0.43
2:O:444:TYR:O	2:O:448:LEU:HD22	2.18	0.43
2:N:193:LEU:O	2:N:198:VAL:HG13	2.18	0.43
2:N:324:PHE:HA	2:N:413:TYR:O	2.19	0.43
1:A:297:GLU:OE1	1:A:398:LYS:NZ	2.42	0.43
1:C:615:LEU:CD2	1:C:615:LEU:C	2.85	0.43
1:D:453:ASN:ND2	1:D:566:ASP:HB3	2.34	0.43
2:M:583:CYS:HB3	2:M:586:THR:HG22	2.00	0.43
2:N:604:ILE:HB	2:N:606:PRO:HD3	2.01	0.43
2:O:487:GLU:O	2:O:490:ASP:CG	2.57	0.43
2:P:504:TYR:CE2	2:P:550:PRO:HB3	2.54	0.43
1:A:186:LEU:HD22	1:A:205:PRO:HD2	2.01	0.43
1:B:414:SER:O	1:B:415:ASN:HB2	2.18	0.43
1:B:661[A]:GLU:CG	1:B:665:ARG:HH21	2.32	0.43
1:C:401:ILE:O	1:C:405:ILE:HG13	2.18	0.43
2:M:244:GLN:HG3	2:M:272:THR:CG2	2.48	0.43
2:N:560:ILE:HD13	2:N:560:ILE:N	2.32	0.43
2:O:373:ILE:HG22	2:O:440:ARG:HG3	1.99	0.43
2:O:51:HIS:HA	2:O:52:PRO:HD3	1.86	0.43
2:O:584:LEU:O	2:O:585:TYR:HD2	2.01	0.43
2:O:657:PHE:O	2:O:658:ILE:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:361:ILE:HG21	2:P:391:TYR:HB2	2.00	0.43
1:B:65:GLY:O	1:B:97:ILE:HG22	2.19	0.43
1:C:557:VAL:CG2	1:C:594:TRP:CZ3	3.02	0.43
2:N:309:ARG:HD2	2:N:309:ARG:HA	1.87	0.43
2:N:604:ILE:HG13	2:N:604:ILE:H	1.57	0.43
2:O:423:ARG:HG2	2:O:423:ARG:HH11	1.84	0.43
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.95	0.43
2:M:335:LYS:HG3	2:M:429:ARG:HH12	1.84	0.43
2:N:441:PHE:CE1	2:N:469:THR:HG21	2.54	0.43
2:O:396:GLN:HG3	2:O:399:PHE:CE1	2.54	0.43
2:P:3:ASP:O	2:P:6:LYS:HB3	2.19	0.43
1:A:537:ILE:HG22	1:A:540:GLY:H	1.84	0.43
1:B:220:HIS:CD2	1:B:221:MET:O	2.71	0.43
1:B:308:LYS:HE3	1:B:308:LYS:HA	2.00	0.43
1:C:164:GLN:O	1:C:168:GLU:HG3	2.18	0.43
1:D:126:GLU:OE1	1:D:390:THR:OG1	2.33	0.43
1:D:28:THR:HG21	1:D:33:VAL:HG12	2.00	0.43
2:O:169:LEU:HD13	2:O:193:LEU:CG	2.49	0.43
2:O:382:LEU:O	2:O:383:PRO:C	2.57	0.43
2:P:79:LEU:HD22	2:P:112:ILE:HG12	2.01	0.43
1:A:12:ARG:NH2	10:A:1449:HOH:O	2.52	0.42
1:C:622:GLN:O	1:C:625:SER:OG	2.30	0.42
1:A:626:ASP:HB3	2:M:212:PHE:CG	2.54	0.42
2:O:390:ILE:HG22	2:O:391:TYR:H	1.84	0.42
1:C:122:HIS:HD2	10:C:869:HOH:O	2.01	0.42
1:C:431:TRP:O	1:C:547:MET:HG2	2.19	0.42
2:N:657:PHE:O	2:N:663:GLY:HA2	2.17	0.42
2:P:356:VAL:HG21	2:P:389:ASP:HB3	2.00	0.42
1:A:220:HIS:CD2	1:A:221:MET:O	2.70	0.42
1:C:216:VAL:HG12	1:D:108:THR:HA	2.00	0.42
2:O:279:ASP:OD1	2:O:279:ASP:C	2.57	0.42
2:O:478:MET:O	2:O:481:ALA:CA	2.67	0.42
2:P:657:PHE:O	2:P:663:GLY:HA2	2.19	0.42
1:A:432:SER:HA	1:A:555:ARG:HD3	2.01	0.42
1:B:515:ASN:HA	1:B:518:THR:CG2	2.47	0.42
1:B:88:GLY:HA3	3:B:750:SF4:S3	2.60	0.42
1:C:196:GLU:OE2	2:O:120:LYS:HE3	2.20	0.42
2:N:354:ARG:HH21	2:N:480:VAL:HG11	1.83	0.42
2:O:459:ILE:HD11	2:O:542:ILE:HG21	1.99	0.42
2:O:482:ARG:HB3	2:O:483:GLU:H	1.67	0.42
2:O:488:ARG:CG	2:O:488:ARG:HH11	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:527:LEU:CD2	2:O:594:SER:HA	2.49	0.42
2:P:372:ASP:OD1	2:P:373:ILE:N	2.42	0.42
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.84	0.42
1:D:201:HIS:CE1	1:D:627:VAL:HG13	2.55	0.42
2:M:247:ARG:NH1	10:M:971:HOH:O	2.52	0.42
2:O:477:TYR:O	2:O:478:MET:C	2.58	0.42
2:O:493:ARG:HH11	2:O:493:ARG:HA	1.84	0.42
1:A:353:VAL:O	1:A:354:GLN:HB2	2.19	0.42
1:B:571:THR:N	1:B:572:PRO:CD	2.83	0.42
1:C:149:ARG:NH1	1:C:149:ARG:HG2	2.34	0.42
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.01	0.42
1:D:573:LYS:HB3	1:D:573:LYS:HE3	1.89	0.42
2:M:138:ASP:N	2:M:139:PRO:CD	2.83	0.42
2:M:702:GLU:H	2:M:702:GLU:HG3	1.30	0.42
2:N:583:CYS:CB	2:N:586:THR:HG22	2.50	0.42
2:P:315:LYS:HE3	10:P:1084:HOH:O	2.19	0.42
1:B:149:ARG:HD2	10:B:1427:HOH:O	2.19	0.42
1:C:577[A]:VAL:HG21	1:C:645:ILE:CG2	2.41	0.42
1:C:213:SER:HB3	1:D:209:HIS:CD2	2.55	0.42
2:M:339:TYR:HB2	2:M:432:LYS:HA	2.02	0.42
2:M:568:ASN:ND2	2:M:581:GLN:HE21	2.14	0.42
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.55	0.42
2:N:377:PRO:HG2	2:N:380:SER:HB3	2.00	0.42
2:O:631:LEU:O	2:O:635:ILE:HG23	2.19	0.42
2:P:117[B]:ARG:NH1	10:P:1004:HOH:O	2.44	0.42
2:P:431:SER:O	2:P:435:VAL:HG23	2.19	0.42
2:P:604:ILE:HD12	2:P:610:GLY:O	2.20	0.42
1:C:368:HIS:CE1	1:C:416:ARG:CB	3.00	0.42
1:C:482:LEU:HD22	1:C:482:LEU:HA	1.81	0.42
1:D:12:ARG:HB3	1:D:13:PRO:HD2	2.02	0.42
2:M:7:ILE:CD1	2:M:245:ARG:HD2	2.43	0.42
2:N:374:ASP:O	2:N:375:GLN:HG3	2.20	0.42
2:N:361:ILE:HD13	2:N:391:TYR:HB3	2.01	0.42
2:N:468:PHE:HB2	2:N:474:VAL:CG2	2.50	0.42
2:N:674:LEU:HD22	2:N:678:LEU:HG	2.01	0.42
2:N:71:GLU:HG2	2:N:82:ILE:HD11	2.02	0.42
1:B:218:GLN:HE22	1:B:233:SER:CB	2.32	0.42
1:B:78:ILE:HD11	1:B:97:ILE:HD12	2.01	0.42
1:C:274:ASP:HB3	1:C:308:LYS:HD3	2.02	0.42
1:D:271:LEU:HD21	1:D:331:VAL:HG11	2.02	0.42
1:D:626:ASP:HB3	2:P:212:PHE:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:298:TYR:HA	2:O:301:ILE:HG13	2.01	0.42
2:O:424:ASN:ND2	2:O:485:TYR:HE1	2.16	0.42
2:O:581:GLN:O	2:O:590:ASN:HB3	2.20	0.42
2:P:542:ILE:HG13	2:P:543:ASN:N	2.35	0.42
2:P:579:LEU:HA	2:P:579:LEU:HD23	1.90	0.42
2:P:728:ILE:HG23	2:P:728:ILE:O	2.20	0.42
2:M:333:ILE:HD12	2:M:418:TRP:CB	2.50	0.41
2:M:424:ASN:H	2:M:424:ASN:ND2	2.14	0.41
2:O:488:ARG:O	2:O:490:ASP:N	2.52	0.41
2:O:584:LEU:O	2:O:585:TYR:CD2	2.72	0.41
2:O:666:ARG:NH2	2:O:725:MET:HE1	2.33	0.41
2:O:95:ASN:ND2	2:O:95:ASN:C	2.74	0.41
2:P:17:GLU:HA	2:P:18:PRO:HD3	1.93	0.41
2:P:422:GLN:HG2	2:P:423:ARG:HG3	2.02	0.41
2:P:594:SER:HB3	2:P:598:PHE:HD2	1.85	0.41
2:P:601:ILE:HG21	2:P:631:LEU:HG	2.01	0.41
1:D:33:VAL:HG13	1:D:339:LEU:CD1	2.49	0.41
1:D:510:LEU:CD1	1:D:510:LEU:H	2.31	0.41
2:N:459:ILE:HD12	2:N:542:ILE:HG13	2.02	0.41
2:N:146:ILE:HD11	3:N:900:SF4:S1	2.60	0.41
2:O:363:ASP:HB2	2:O:462:ARG:HG2	2.03	0.41
2:O:474:VAL:CG1	2:O:475:LYS:N	2.83	0.41
2:P:500:VAL:O	2:P:553:LYS:NZ	2.47	0.41
2:P:541:GLU:HG2	2:P:541:GLU:H	1.56	0.41
1:A:200:THR:OG1	1:A:201:HIS:HD2	2.03	0.41
1:A:217:ASN:O	1:A:223:MET:HG3	2.21	0.41
1:D:615:LEU:H	5:D:863:GOL:H12	1.84	0.41
2:M:277:ILE:HG23	2:M:295:VAL:HG23	2.02	0.41
2:O:167:LYS:HG2	10:O:997:HOH:O	2.20	0.41
2:O:315:LYS:HB2	2:O:316:ILE:H	1.50	0.41
2:O:430:VAL:CG1	2:O:431:SER:H	2.32	0.41
2:O:552:PRO:O	2:O:554:GLU:N	2.49	0.41
2:O:671:PRO:HA	2:O:702:GLU:OE1	2.20	0.41
2:P:392:GLY:HA3	2:P:459:ILE:O	2.20	0.41
2:P:505:SER:CB	2:P:570:TYR:HE2	2.31	0.41
2:P:704:ILE:HG22	2:P:711:ILE:HG22	2.02	0.41
1:B:186:LEU:CD2	1:B:205:PRO:HD2	2.50	0.41
1:D:69:ARG:HD3	1:D:75:PRO:HG3	2.02	0.41
2:M:21:LEU:HB2	2:M:286:LYS:HA	2.03	0.41
2:N:16:LYS:HB3	2:N:16:LYS:HZ3	1.85	0.41
2:N:156:GLU:HG3	2:N:182:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:696:ILE:HA	2:N:699:ILE:HD12	2.02	0.41
2:O:249:ARG:HA	2:O:309:ARG:NH2	2.36	0.41
2:O:396:GLN:NE2	2:O:399:PHE:HD1	2.12	0.41
2:O:427:TRP:CE2	2:O:429:ARG:NH2	2.88	0.41
2:O:388:VAL:HG22	2:O:465:VAL:HG13	2.01	0.41
2:O:527:LEU:HD22	2:O:594:SER:HA	2.00	0.41
2:O:95:ASN:HD21	2:O:98:ASN:H	1.67	0.41
1:C:577[A]:VAL:HG12	1:C:601:PRO:HG2	2.01	0.41
1:D:510:LEU:O	1:D:543:PRO:HD2	2.21	0.41
2:O:271:PHE:CD2	2:O:271:PHE:C	2.94	0.41
2:O:348:PRO:CG	2:O:475:LYS:HE3	2.46	0.41
2:O:666:ARG:CZ	2:O:725:MET:HE2	2.43	0.41
2:O:728:ILE:O	2:O:729:MET:O	2.38	0.41
1:B:118:ASN:HD22	1:B:118:ASN:C	2.23	0.41
1:B:160:LEU:HA	1:B:160:LEU:HD23	1.87	0.41
1:C:169:LYS:O	1:C:172:GLU:HB2	2.21	0.41
1:C:61:ILE:HG22	1:C:67:CYS:HB2	2.02	0.41
2:O:360:GLU:O	2:O:361:ILE:CG2	2.68	0.41
2:O:712:LEU:O	2:O:715:LEU:N	2.54	0.41
2:P:478:MET:O	2:P:482:ARG:HB2	2.20	0.41
1:B:368:HIS:NE2	1:B:416:ARG:CD	2.84	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.21	0.41
1:C:235:ILE:HG23	1:C:597:SER:OG	2.21	0.41
2:N:350:PHE:HA	2:N:423:ARG:O	2.20	0.41
2:O:482:ARG:O	2:O:485:TYR:HB3	2.20	0.41
2:P:254:TYR:O	2:P:278:THR:HA	2.21	0.41
2:P:581:GLN:O	2:P:590:ASN:HB3	2.20	0.41
1:B:467:ILE:O	1:B:497:ALA:HA	2.20	0.41
1:C:507:LYS:HB2	1:C:507:LYS:HE3	1.87	0.41
1:D:186:LEU:HD22	1:D:205:PRO:HD2	2.03	0.41
2:M:315:LYS:O	2:M:316:ILE:O	2.38	0.41
2:M:683:VAL:HG13	2:M:693:GLU:HA	2.03	0.41
2:O:482:ARG:O	2:O:485:TYR:CB	2.69	0.41
2:M:169:LEU:HD13	2:M:193:LEU:HD21	2.03	0.41
2:O:344:GLY:N	2:O:426:ASN:O	2.54	0.41
2:O:661:ASP:O	2:O:666:ARG:NE	2.32	0.41
2:P:656:LYS:HA	2:P:656:LYS:HD3	1.81	0.41
1:D:149[B]:ARG:HD2	1:D:188:THR:O	2.20	0.41
2:O:488:ARG:CG	2:O:488:ARG:NH1	2.83	0.41
2:O:604:ILE:CD1	2:O:606:PRO:HD3	2.30	0.41
1:A:587:LYS:H	1:B:220:HIS:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HD11	1:A:97:ILE:HD12	2.03	0.41
1:B:601:PRO:HB3	1:B:631:TYR:CZ	2.56	0.41
1:C:313:VAL:HG12	1:C:329:PRO:HG2	2.02	0.41
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.85	0.41
2:O:653:VAL:C	2:O:685:ARG:HD2	2.39	0.41
2:O:726:ASP:HB2	2:O:727:PRO:HD2	2.03	0.41
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.85	0.41
1:A:279:VAL:HG22	1:A:313:VAL:CG2	2.51	0.40
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.33	0.40
1:C:197:LYS:HE2	1:C:197:LYS:HB2	1.88	0.40
1:D:220:HIS:CD2	1:D:221:MET:O	2.72	0.40
2:M:477:TYR:C	2:M:479:GLU:H	2.25	0.40
2:M:711:ILE:O	2:M:715:LEU:HG	2.20	0.40
2:N:651:TYR:HA	10:N:876:HOH:O	2.21	0.40
2:O:182:MET:HG3	2:O:205:ILE:HG22	2.01	0.40
2:O:281:PRO:HG3	2:O:296:GLU:OE2	2.21	0.40
2:O:396:GLN:CD	2:O:399:PHE:HD1	2.25	0.40
2:O:351:GLU:CG	2:O:423:ARG:N	2.65	0.40
2:O:430:VAL:HG12	2:O:434:ALA:HB3	2.03	0.40
2:O:61:TYR:CD1	2:O:66:ARG:HD2	2.55	0.40
5:D:863:GOL:C2	2:P:27:HIS:CE1	3.00	0.40
2:P:21:LEU:HB2	2:P:286:LYS:HA	2.01	0.40
2:P:494:GLY:N	10:P:1094:HOH:O	2.34	0.40
1:A:235:ILE:HG23	1:A:597:SER:OG	2.21	0.40
1:A:77:ARG:HB3	10:A:1466:HOH:O	2.22	0.40
2:O:351:GLU:O	2:O:352:LEU:CB	2.65	0.40
2:O:366:ILE:HG13	2:O:366:ILE:H	1.74	0.40
2:P:341:GLU:OE1	2:P:427:TRP:NE1	2.53	0.40
1:B:652:ARG:O	1:B:656:LEU:HB2	2.22	0.40
1:D:170:ALA:O	1:D:173:ASP:HB2	2.21	0.40
1:D:201:HIS:HE1	1:D:627:VAL:HG13	1.86	0.40
2:M:199:LYS:HE2	2:M:415:GLU:OE2	2.22	0.40
2:M:563:ILE:HD11	2:M:583:CYS:SG	2.61	0.40
2:O:111:GLU:HA	2:O:216:VAL:HG11	2.03	0.40
2:P:287:GLN:HE22	2:P:289:PRO:HG3	1.87	0.40
1:C:174:PHE:CE2	1:C:208:ILE:HD12	2.56	0.40
1:D:200:THR:OG1	1:D:201:HIS:HD2	2.05	0.40
2:M:349:ALA:CB	2:M:426:ASN:HD21	2.35	0.40
1:B:662:VAL:HG21	2:N:194:LEU:HD13	2.03	0.40
2:N:602:MET:HE2	2:N:602:MET:HB3	1.98	0.40
2:N:604:ILE:HG13	2:N:643:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:484:LYS:HA	2:O:484:LYS:HD3	1.59	0.40
1:A:20:MET:HG3	10:A:883:HOH:O	2.21	0.40
1:A:440:LEU:HB3	1:A:448:PRO:O	2.21	0.40
1:C:384:TYR:HE2	2:P:88:ALA:HB2	1.86	0.40
2:M:349:ALA:HB3	2:M:426:ASN:HD21	1.86	0.40
2:O:720:HIS:O	2:O:723:LEU:N	2.54	0.40
2:P:442:LYS:HB2	2:P:442:LYS:HE2	1.66	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	678/674 (101%)	652 (96%)	24 (4%)	2 (0%)	41	37
1	B	676/674 (100%)	652 (96%)	23 (3%)	1 (0%)	51	53
1	C	673/674 (100%)	648 (96%)	24 (4%)	1 (0%)	51	53
1	D	675/674 (100%)	640 (95%)	30 (4%)	5 (1%)	22	15
2	M	731/729 (100%)	687 (94%)	36 (5%)	8 (1%)	14	8
2	N	732/729 (100%)	689 (94%)	34 (5%)	9 (1%)	13	7
2	O	727/729 (100%)	641 (88%)	60 (8%)	26 (4%)	3	0
2	P	727/729 (100%)	679 (93%)	41 (6%)	7 (1%)	15	9
All	All	5619/5612 (100%)	5288 (94%)	272 (5%)	59 (1%)	14	8

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	D	267	ASN
2	M	316	ILE

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Mol	Chain	Res	Type
2	M	693	GLU
2	O	315	LYS
2	O	316	ILE
2	O	317	LYS
2	O	361	ILE
2	O	397	ALA
2	O	482	ARG
2	O	485	TYR
2	O	486	LYS
2	O	492	MET
2	O	728	ILE
2	P	316	ILE
2	P	360	GLU
1	A	267	ASN
2	M	187	ASP
2	M	315	LYS
2	N	187	ASP
2	N	449	VAL
2	N	693	GLU
2	O	187	ASP
2	O	335	LYS
2	O	470	ASP
2	O	555	GLY
2	P	458	ALA
2	P	679	HIS
1	C	267	ASN
2	M	596	GLY
2	M	658	ILE
2	O	436	ALA
2	O	489	ASP
2	O	650	THR
2	O	679	HIS
2	P	187	ASP
2	N	426	ASN
2	O	399	PHE
2	P	228	MET
2	P	596	GLY
1	A	354	GLN
1	D	552	ASP
2	N	290	ASP
2	O	459	ILE
2	O	727	PRO

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Mol	Chain	Res	Type
1	D	354	GLN
1	D	416	ARG
1	D	492	ASN
2	M	478	MET
2	M	719	GLY
2	N	596	GLY
2	O	484	LYS
2	N	316	ILE
2	O	382	LEU
2	O	460	VAL
2	N	402	VAL
2	O	392	GLY
2	O	658	ILE
2	N	658	ILE

### 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	548/543 (101%)	524 (96%)	24 (4%)	28	25
1	B	547/543 (101%)	529 (97%)	18 (3%)	38	37
1	C	542/543 (100%)	521 (96%)	21 (4%)	32	30
1	D	544/543 (100%)	525 (96%)	19 (4%)	36	34
2	M	615/611 (101%)	570 (93%)	45 (7%)	14	9
2	N	615/611 (101%)	574 (93%)	41 (7%)	16	11
2	O	611/611 (100%)	532 (87%)	79 (13%)	4	1
2	P	611/611 (100%)	550 (90%)	61 (10%)	7	4
All	All	4633/4616 (100%)	4325 (93%)	308 (7%)	16	11

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG

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Mol	Chain	Res	Type
1	A	31	PRO
1	A	118	ASN
1	A	153	GLU
1	A	206	PHE
1	A	284	ASN
1	A	303	LYS
1	A	318	THR
1	A	415	ASN
1	A	418	VAL
1	A	426	ARG
1	A	427	VAL
1	A	438	LYS
1	A	482	LEU
1	A	518	THR
1	A	536	ASN
1	A	538	GLU
1	A	546	HIS
1	A	647	ASP
1	A	655	LYS
1	A	656	LEU
1	A	664	GLU
1	A	665[A]	ARG
1	A	665[B]	ARG
1	B	66	ILE
1	B	77	ARG
1	B	118	ASN
1	B	120	ILE
1	B	153	GLU
1	B	159	VAL
1	B	206	PHE
1	B	308	LYS
1	B	395	GLU
1	B	411	ARG
1	B	413	GLU
1	B	447	ASN
1	B	482	LEU
1	B	518	THR
1	B	537	ILE
1	B	636	MET
1	B	647	ASP
1	B	656	LEU
1	C	23	LYS

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Mol	Chain	Res	Type
1	C	27	ARG
1	C	81	THR
1	C	82	ASP
1	C	118	ASN
1	C	159	VAL
1	C	206	PHE
1	C	359	SER
1	C	390	THR
1	C	395	GLU
1	C	482	LEU
1	C	539	ILE
1	C	546	HIS
1	C	576	PHE
1	C	600	VAL
1	C	636	MET
1	C	639	GLN
1	C	647	ASP
1	C	656	LEU
1	C	664	GLU
1	C	669	LYS
1	D	45	VAL
1	D	66	ILE
1	D	118	ASN
1	D	153	GLU
1	D	159	VAL
1	D	190	ILE
1	D	196	GLU
1	D	199	ARG
1	D	206	PHE
1	D	284	ASN
1	D	293	GLN
1	D	299	GLU
1	D	331	VAL
1	D	466	LEU
1	D	467	ILE
1	D	546	HIS
1	D	594	TRP
1	D	656	LEU
1	D	664	GLU
2	M	6[A]	LYS
2	M	6[B]	LYS
2	M	14	GLU

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Mol	Chain	Res	Type
2	M	66	ARG
2	M	125	GLU
2	M	169	LEU
2	M	198	VAL
2	M	199	LYS
2	M	215	ILE
2	M	245	ARG
2	M	254	TYR
2	M	262	LYS
2	M	314	THR
2	M	317	LYS
2	M	318	LEU
2	M	332	SER
2	M	335	LYS
2	M	342	MET
2	M	354	ARG
2	M	373	ILE
2	M	376	ILE
2	M	380	SER
2	M	409	ASP
2	M	422	GLN
2	M	424	ASN
2	M	426	ASN
2	M	448	LEU
2	M	469	THR
2	M	475	LYS
2	M	486	LYS
2	M	539	SER
2	M	571	LEU
2	M	598	PHE
2	M	604	ILE
2	M	607	GLU
2	M	612	MET
2	M	654	SER
2	M	672	LYS
2	M	674	LEU
2	M	684	ARG
2	M	694	ASP
2	M	702	GLU
2	M	704	ILE
2	M	724	THR
2	M	726	ASP

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Mol	Chain	Res	Type
2	N	66	ARG
2	N	96	PHE
2	N	124	ASP
2	N	125	GLU
2	N	152	THR
2	N	174[A]	LYS
2	N	174[B]	LYS
2	N	198	VAL
2	N	245	ARG
2	N	254	TYR
2	N	312	LYS
2	N	313	LEU
2	N	315	LYS
2	N	316	ILE
2	N	331	GLU
2	N	335	LYS
2	N	338	MET
2	N	342	MET
2	N	354	ARG
2	N	358	GLU
2	N	373	ILE
2	N	386	ILE
2	N	405	ARG
2	N	424	ASN
2	N	425	ILE
2	N	440	ARG
2	N	448	LEU
2	N	471	GLU
2	N	492	MET
2	N	493	ARG
2	N	495	LEU
2	N	560	ILE
2	N	571	LEU
2	N	598	PHE
2	N	604	ILE
2	N	606	PRO
2	N	631	LEU
2	N	674	LEU
2	N	681	GLU
2	N	686	SER
2	N	702	GLU
2	O	6	LYS

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Mol	Chain	Res	Type
2	O	39	LEU
2	O	66	ARG
2	O	95	ASN
2	O	96	PHE
2	O	125	GLU
2	O	127	LEU
2	O	149	VAL
2	O	152	THR
2	O	166	SER
2	O	169	LEU
2	O	205	ILE
2	O	208	PRO
2	O	216	VAL
2	O	233	THR
2	O	238	GLU
2	O	245	ARG
2	O	271	PHE
2	O	313	LEU
2	O	314	THR
2	O	316	ILE
2	O	317	LYS
2	O	318	LEU
2	O	322	ILE
2	O	333	ILE
2	O	335	LYS
2	O	339	TYR
2	O	342	MET
2	O	350	PHE
2	O	351	GLU
2	O	352	LEU
2	O	368	VAL
2	O	391	TYR
2	O	395	MET
2	O	404	GLU
2	O	407	ILE
2	O	411	ILE
2	O	426	ASN
2	O	427	TRP
2	O	429	ARG
2	O	442	LYS
2	O	448	LEU
2	O	453	LYS

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Mol	Chain	Res	Type
2	O	454	GLU
2	O	459	ILE
2	O	463	VAL
2	O	478	MET
2	O	480	VAL
2	O	482	ARG
2	O	484	LYS
2	O	487	GLU
2	O	491	ARG
2	O	492	MET
2	O	493	ARG
2	O	495	LEU
2	O	497	ASP
2	O	499	THR
2	O	524	ARG
2	O	541	GLU
2	O	542	ILE
2	O	556	GLU
2	O	573	THR
2	O	575	SER
2	O	579	LEU
2	O	580	GLU
2	O	598	PHE
2	O	608	CYS
2	O	612	MET
2	O	621	MET
2	O	631	LEU
2	O	647	ILE
2	O	659	SER
2	O	672	LYS
2	O	686	SER
2	O	691	LEU
2	O	693	GLU
2	O	696	ILE
2	O	697	ASP
2	O	729	MET
2	P	39	LEU
2	P	96	PHE
2	P	124	ASP
2	P	152	THR
2	P	166	SER
2	P	174	LYS

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Mol	Chain	Res	Type
2	P	175	GLU
2	P	198	VAL
2	P	199	LYS
2	P	238	GLU
2	P	245	ARG
2	P	254	TYR
2	P	284	GLU
2	P	300	LYS
2	P	312	LYS
2	P	317	LYS
2	P	331	GLU
2	P	332	SER
2	P	335	LYS
2	P	341	GLU
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	351	GLU
2	P	354	ARG
2	P	362	THR
2	P	369	ILE
2	P	373	ILE
2	P	398	ASP
2	P	404	GLU
2	P	409	ASP
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	440	ARG
2	P	442	LYS
2	P	448	LEU
2	P	462	ARG
2	P	467	ILE
2	P	469	THR
2	P	480	VAL
2	P	482	ARG
2	P	483	GLU
2	P	486	LYS
2	P	491	ARG
2	P	498	GLU
2	P	500	VAL
2	P	502	THR

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Mol	Chain	Res	Type
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	549	GLN
2	P	581	GLN
2	P	605	LEU
2	P	631	LEU
2	P	655	LYS
2	P	674	LEU
2	P	686	SER
2	P	717	GLU
2	P	726	ASP
2	P	729	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	201	HIS
1	A	209	HIS
1	A	217	ASN
1	A	218	GLN
1	A	220	HIS
1	A	284	ASN
1	A	471	ASN
1	A	477	GLN
1	A	503	GLN
1	A	515	ASN
1	A	622	GLN
1	B	9	HIS
1	B	122	HIS
1	B	201	HIS
1	B	209	HIS
1	B	217	ASN
1	B	218	GLN
1	B	220	HIS
1	B	260	GLN
1	B	293	GLN
1	B	454	GLN
1	B	477	GLN
1	B	672	GLN
1	C	9	HIS

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Mol	Chain	Res	Type
1	C	164	GLN
1	C	201	HIS
1	C	209	HIS
1	C	217	ASN
1	C	218	GLN
1	C	220	HIS
1	C	368	HIS
1	C	454	GLN
1	C	503	GLN
1	C	515	ASN
1	D	201	HIS
1	D	209	HIS
1	D	217	ASN
1	D	218	GLN
1	D	220	HIS
1	D	260	GLN
1	D	284	ASN
1	D	477	GLN
1	D	622	GLN
2	M	211	ASN
2	M	375	GLN
2	M	408	HIS
2	M	424	ASN
2	M	426	ASN
2	M	544	HIS
2	M	581	GLN
2	M	590	ASN
2	N	211	ASN
2	N	345	ASN
2	N	408	HIS
2	N	424	ASN
2	N	510	GLN
2	N	581	GLN
2	N	590	ASN
2	N	640	GLN
2	O	27	HIS
2	O	95	ASN
2	O	211	ASN
2	O	419	HIS
2	O	516	HIS
2	O	549	GLN
2	O	568	ASN

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Mol	Chain	Res	Type
2	O	578	ASN
2	P	27	HIS
2	P	211	ASN
2	P	287	GLN
2	P	408	HIS
2	P	422	GLN
2	P	424	ASN
2	P	426	ASN
2	P	516	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 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	$\# Z  > 2$
5	GOL	A	863	-	5,5,5	0.44	0	5,5,5	1.69	1 (20%)
8	ACT	P	953	-	1,2,3	1.47	0	1,1,3	0.23	0
5	GOL	B	863	-	5,5,5	1.08	1 (20%)	5,5,5	1.73	1 (20%)
3	SF4	N	900	2	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	M	900	2	0,12,12	0.00	-	-		
5	GOL	D	863	-	5,5,5	0.51	0	5,5,5	1.60	1 (20%)
8	ACT	O	953	-	1,2,3	1.17	0	1,1,3	0.47	0
5	GOL	C	863	-	5,5,5	0.30	0	5,5,5	0.62	0
3	SF4	C	750	1	0,12,12	0.00	-	-		
8	ACT	M	953	-	1,2,3	1.29	0	1,1,3	0.75	0
4	XCC	A	800	1,10	0,11,11	0.00	-	-		
3	SF4	B	750	1	0,12,12	0.00	-	-		
3	SF4	D	750	1	0,12,12	0.00	-	-		
8	ACT	N	953	-	1,2,3	1.38	0	1,1,3	0.10	0
3	SF4	P	900	2	0,12,12	0.00	-	-		
3	SF4	A	750	1	0,12,12	0.00	-	-		
3	SF4	O	900	2	0,12,12	0.00	-	-		
4	XCC	D	800	1,10	0,11,11	0.00	-	-		
3	SF4	C	700	1	0,12,12	0.00	-	-		
3	SF4	A	700	1	0,12,12	0.00	-	-		
4	XCC	B	800	1,10	0,11,11	0.00	-	-		
4	XCC	C	800	1,10	0,11,11	0.00	-	-		

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
5	GOL	A	863	-	-	2/4/4/4	-
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	D	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	M	900	2	-	-	0/6/5/5
5	GOL	B	863	-	-	0/4/4/4	-
3	SF4	N	900	2	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
4	XCC	B	800	1,10	-	-	0/3/3/3
5	GOL	D	863	-	-	3/4/4/4	-
4	XCC	C	800	1,10	-	-	0/3/3/3
4	XCC	A	800	1,10	-	-	0/3/3/3
4	XCC	D	800	1,10	-	-	0/3/3/3
5	GOL	C	863	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	700	1	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	863	GOL	O2-C2	-2.36	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	863	GOL	O2-C2-C3	-3.08	95.57	109.12
5	D	863	GOL	O1-C1-C2	-2.66	97.45	110.20
5	A	863	GOL	O1-C1-C2	-2.30	99.16	110.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	863	GOL	O1-C1-C2-C3
5	C	863	GOL	O1-C1-C2-C3
5	D	863	GOL	O1-C1-C2-C3
5	C	863	GOL	O1-C1-C2-O2
5	D	863	GOL	O1-C1-C2-O2
5	A	863	GOL	O1-C1-C2-O2
5	D	863	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	P	953	ACT	1	0
3	N	900	SF4	1	0
5	D	863	GOL	6	0
8	O	953	ACT	1	0
5	C	863	GOL	5	0
3	B	750	SF4	1	0
3	O	900	SF4	2	0
4	D	800	XCC	2	0
3	C	700	SF4	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	673/674 (99%)	-0.19	8 (1%) 79 83	14, 25, 43, 60	0
1	B	673/674 (99%)	-0.18	8 (1%) 79 83	13, 22, 39, 68	0
1	C	673/674 (99%)	-0.27	8 (1%) 79 83	19, 28, 42, 58	0
1	D	673/674 (99%)	-0.16	14 (2%) 63 71	21, 31, 45, 59	0
2	M	728/729 (99%)	-0.13	8 (1%) 80 85	16, 33, 62, 74	0
2	N	728/729 (99%)	-0.07	17 (2%) 60 68	15, 32, 66, 76	0
2	O	728/729 (99%)	1.77	278 (38%) 0 0	26, 64, 92, 126	0
2	P	728/729 (99%)	0.43	90 (12%) 4 5	22, 45, 76, 92	0
All	All	5604/5612 (99%)	0.16	431 (7%) 13 18	13, 31, 74, 126	0

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	458	ALA	11.9
2	O	474	VAL	10.9
2	O	471	GLU	9.8
2	O	485	TYR	9.5
2	O	457	PRO	9.3
2	O	397	ALA	9.1
2	O	470	ASP	9.1
2	O	481	ALA	8.9
2	O	574	ALA	7.7
2	O	428	LEU	7.7
2	O	333	ILE	7.6
2	O	724	THR	7.3
2	O	469	THR	7.2
2	O	486	LYS	7.2
2	O	359	SER	7.1
2	O	357	SER	7.0

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Mol	Chain	Res	Type	RSRZ
2	O	348	PRO	6.9
2	O	492	MET	6.8
2	O	354	ARG	6.7
2	O	356	VAL	6.7
2	O	373	ILE	6.6
2	O	567	VAL	6.5
2	O	369	ILE	6.5
2	O	477	TYR	6.5
2	O	692	GLY	6.4
2	O	391	TYR	6.4
2	O	475	LYS	6.3
2	O	392	GLY	6.2
2	O	380	SER	6.1
2	O	418	TRP	6.1
2	O	379	GLY	6.1
2	O	361	ILE	6.1
2	O	493	ARG	6.1
2	O	339	TYR	6.0
2	O	436	ALA	5.9
2	O	572	TYR	5.9
2	O	664	ILE	5.9
2	O	564	TRP	5.8
2	O	344	GLY	5.8
2	O	559	PRO	5.8
2	O	557	ILE	5.8
2	O	687	VAL	5.7
2	O	715	LEU	5.7
2	O	353	VAL	5.7
2	O	426	ASN	5.7
2	O	483	GLU	5.7
2	O	723	LEU	5.7
2	O	364	GLY	5.6
2	O	697	ASP	5.6
2	O	542	ILE	5.6
2	O	690	GLY	5.5
2	M	314	THR	5.5
2	O	399	PHE	5.5
2	O	461	ASP	5.5
2	O	468	PHE	5.4
2	O	560	ILE	5.4
2	O	685	ARG	5.4
2	O	576	ASN	5.4

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Mol	Chain	Res	Type	RSRZ
2	O	314	THR	5.3
2	O	402	VAL	5.3
2	O	316	ILE	5.3
2	O	729	MET	5.3
2	O	552	PRO	5.3
2	O	374	ASP	5.3
2	O	350	PHE	5.2
2	O	384	LEU	5.2
2	P	483	GLU	5.2
2	O	345	ASN	5.2
2	P	359	SER	5.1
2	O	684	ARG	5.1
2	N	468	PHE	5.1
2	O	639	THR	5.1
2	O	577	ARG	5.0
2	O	714	TYR	5.0
2	O	387	LEU	5.0
2	O	124	ASP	5.0
2	O	424	ASN	5.0
2	O	451	LYS	4.9
2	O	696	ILE	4.9
2	O	15	GLY	4.9
2	O	728	ILE	4.9
2	O	504	TYR	4.9
2	O	712	LEU	4.9
2	O	472	ALA	4.9
2	O	570	TYR	4.9
2	P	552	PRO	4.9
2	P	425	ILE	4.8
2	O	494	GLY	4.8
2	O	563	ILE	4.7
2	O	449	VAL	4.7
2	O	482	ARG	4.7
2	O	573	THR	4.7
2	O	382	LEU	4.7
2	O	394	LYS	4.7
2	O	479	GLU	4.7
2	O	543	ASN	4.7
2	P	486	LYS	4.7
2	O	498	GLU	4.6
2	O	395	MET	4.6
2	O	420	THR	4.6

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Mol	Chain	Res	Type	RSRZ
2	O	14	GLU	4.6
2	O	709	ASP	4.6
2	O	555	GLY	4.6
2	O	362	THR	4.6
2	O	2	THR	4.5
2	P	481	ALA	4.5
2	O	478	MET	4.5
1	B	539	ILE	4.5
2	O	716	GLU	4.5
2	O	421	GLY	4.5
2	P	565	LYS	4.4
2	O	401	GLY	4.4
2	O	463	VAL	4.4
2	O	476	GLU	4.3
2	O	381	LYS	4.3
2	O	342	MET	4.3
2	O	335	LYS	4.3
2	O	349	ALA	4.3
2	O	717	GLU	4.3
2	P	493	ARG	4.3
2	O	695	PHE	4.3
2	O	683	VAL	4.3
2	O	554	GLU	4.2
2	O	473	LYS	4.2
2	N	729	MET	4.2
2	P	393	ARG	4.2
2	O	699	ILE	4.1
2	P	361	ILE	4.1
2	O	393	ARG	4.1
1	A	415	ASN	4.1
2	O	423	ARG	4.1
2	O	655	LYS	4.1
2	O	704	ILE	4.1
2	O	713	PRO	4.1
2	P	358	GLU	4.1
2	O	462	ARG	4.1
2	O	571	LEU	4.1
2	O	407	ILE	4.1
2	O	453	LYS	4.1
2	O	396	GLN	4.1
2	O	459	ILE	4.1
2	O	422	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
2	O	425	ILE	4.0
2	O	653	VAL	3.9
2	P	729	MET	3.9
2	O	3	ASP	3.9
2	O	434	ALA	3.9
2	P	461	ASP	3.9
2	O	454	GLU	3.9
2	O	691	LEU	3.9
2	O	688	GLU	3.9
2	O	679	HIS	3.9
2	P	474	VAL	3.8
2	P	551	ILE	3.8
2	P	480	VAL	3.8
2	O	343	GLY	3.8
2	P	369	ILE	3.8
2	O	355	THR	3.8
2	O	366	ILE	3.7
2	O	669	TRP	3.7
2	P	391	TYR	3.7
2	N	348	PRO	3.7
2	O	668	VAL	3.7
2	O	689	GLU	3.7
2	O	566	SER	3.7
2	O	694	ASP	3.7
2	P	623	PRO	3.7
2	P	490	ASP	3.7
2	O	460	VAL	3.7
2	O	544	HIS	3.6
2	O	467	ILE	3.6
2	O	682	PHE	3.6
2	O	726	ASP	3.6
2	O	334	ARG	3.6
2	O	388	VAL	3.6
2	O	389	ASP	3.6
2	P	492	MET	3.6
2	O	545	ALA	3.6
2	O	6	LYS	3.6
2	O	442	LYS	3.6
2	P	314	THR	3.6
2	P	712	LEU	3.6
2	O	721	PRO	3.6
1	D	415	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
2	O	499	THR	3.5
2	O	319	ASP	3.5
2	O	676	ASP	3.5
2	O	427	TRP	3.5
2	O	435	VAL	3.5
2	O	558	ASP	3.5
2	O	578	ASN	3.5
2	O	638	GLY	3.5
2	O	465	VAL	3.5
2	O	583	CYS	3.5
1	D	417	PRO	3.5
2	P	577	ARG	3.5
2	P	392	GLY	3.5
2	O	360	GLU	3.5
2	O	390	ILE	3.4
2	O	605	LEU	3.4
2	P	124	ASP	3.4
2	O	693	GLU	3.4
2	O	540	TYR	3.3
2	P	572	TYR	3.3
2	O	377	PRO	3.3
2	O	383	PRO	3.3
2	P	16	LYS	3.3
2	O	575	SER	3.3
2	O	318	LEU	3.3
2	O	376	ILE	3.3
2	O	507	VAL	3.3
2	P	475	LYS	3.3
2	O	490	ASP	3.3
2	O	346	ARG	3.3
2	O	336	GLY	3.3
2	O	662	GLY	3.3
2	O	363	ASP	3.3
2	O	317	LYS	3.3
2	O	580	GLU	3.2
1	D	413	GLU	3.2
2	O	487	GLU	3.2
2	O	332	SER	3.2
2	O	502	THR	3.2
1	B	537	ILE	3.2
2	O	340	VAL	3.2
2	O	433	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	570	TYR	3.2
2	P	14	GLU	3.2
2	O	484	LYS	3.2
2	O	727	PRO	3.1
2	P	485	TYR	3.1
2	O	375	GLN	3.1
2	P	470	ASP	3.1
2	O	614	THR	3.1
2	N	361	ILE	3.1
2	N	490	ASP	3.1
2	P	557	ILE	3.1
2	O	623	PRO	3.1
2	O	635	ILE	3.1
2	P	350	PHE	3.1
2	P	684	ARG	3.1
1	C	416	ARG	3.1
2	O	533	TRP	3.0
2	O	637	GLY	3.0
2	P	335	LYS	3.0
2	P	727	PRO	3.0
2	O	489	ASP	3.0
2	O	497	ASP	3.0
2	O	565	LYS	3.0
2	O	725	MET	3.0
2	P	477	TYR	3.0
1	D	416	ARG	3.0
2	N	472	ALA	3.0
2	O	400	GLU	3.0
2	O	672	LYS	3.0
2	O	347	THR	2.9
2	O	710	GLU	2.9
2	M	124	ASP	2.9
1	B	538	GLU	2.9
2	O	541	GLU	2.9
2	P	356	VAL	2.9
2	O	441	PHE	2.9
2	O	718	LYS	2.9
2	O	608	CYS	2.9
2	N	124	ASP	2.9
2	O	569	ASP	2.9
2	O	703	THR	2.9
2	P	573	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	659	SER	2.9
2	N	373	ILE	2.8
2	O	711	ILE	2.8
2	M	693	GLU	2.8
2	P	479	GLU	2.8
2	O	440	ARG	2.8
2	O	707	THR	2.8
1	B	536	ASN	2.8
2	O	358	GLU	2.8
2	P	499	THR	2.8
2	O	438	GLY	2.8
1	D	466	LEU	2.8
2	O	517	VAL	2.7
2	O	352	LEU	2.7
2	P	576	ASN	2.7
1	B	416	ARG	2.7
2	N	314	THR	2.7
2	O	16	LYS	2.7
2	O	338	MET	2.7
1	C	415	ASN	2.7
2	O	378	GLU	2.7
2	P	427	TRP	2.7
1	C	468	CYS	2.7
2	O	706	THR	2.7
2	O	621	MET	2.7
2	O	480	VAL	2.7
2	M	481	ALA	2.7
2	P	696	ILE	2.6
2	O	488	ARG	2.6
2	O	657	PHE	2.6
2	O	626	MET	2.6
2	O	681	GLU	2.6
2	P	472	ALA	2.6
2	O	634	MET	2.6
2	O	123	PRO	2.6
2	O	551	ILE	2.6
2	P	488	ARG	2.6
2	P	15	GLY	2.6
2	O	579	LEU	2.6
2	P	564	TRP	2.6
2	O	337	ASP	2.6
1	D	368	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	642	PRO	2.6
2	O	702	GLU	2.6
2	O	372	ASP	2.5
2	O	686	SER	2.5
2	P	707	THR	2.5
2	O	447	ILE	2.5
2	P	693	GLU	2.5
2	P	363	ASP	2.5
2	N	318	LEU	2.5
2	P	216	VAL	2.5
2	N	339	TYR	2.5
2	N	493	ARG	2.5
2	O	625	GLY	2.5
2	O	658	ILE	2.5
2	N	684	ARG	2.5
2	O	663	GLY	2.5
2	P	555	GLY	2.5
2	O	678	LEU	2.4
2	P	687	VAL	2.4
2	P	484	LYS	2.4
2	P	559	PRO	2.4
2	O	556	GLU	2.4
2	P	215	ILE	2.4
2	O	437	LYS	2.4
2	O	534	LEU	2.4
1	A	300	GLY	2.4
2	P	638	GLY	2.4
2	P	345	ASN	2.4
2	O	613	ILE	2.4
1	B	316	CYS	2.4
2	O	320	LEU	2.4
2	O	587	LEU	2.4
2	P	487	GLU	2.4
2	O	708	VAL	2.4
2	O	515	ASN	2.4
2	P	218	ALA	2.4
1	D	468	CYS	2.3
1	C	466	LEU	2.3
2	O	640	GLN	2.3
2	O	4	PHE	2.3
2	P	418	TRP	2.3
2	M	472	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	538	ALA	2.3
1	C	591	ILE	2.3
2	P	688	GLU	2.3
2	P	355	THR	2.3
2	O	429	ARG	2.3
2	M	14	GLU	2.3
2	O	439	PHE	2.3
2	O	450	ALA	2.3
2	O	632	ALA	2.3
1	A	309	GLY	2.3
1	A	155	GLU	2.3
2	O	667	ILE	2.3
2	P	284	GLU	2.3
2	O	603	ALA	2.2
2	P	468	PHE	2.2
2	O	351	GLU	2.2
2	P	432	LYS	2.2
2	O	680	ASP	2.2
2	P	3	ASP	2.2
2	P	574	ALA	2.2
2	O	503	PHE	2.2
2	M	316	ILE	2.2
2	O	722	ALA	2.2
2	P	362	THR	2.2
2	P	364	GLY	2.2
1	D	15	GLU	2.2
2	O	581	GLN	2.2
2	P	482	ARG	2.2
2	O	416	GLY	2.2
2	O	606	PRO	2.2
2	P	340	VAL	2.2
2	P	6	LYS	2.2
2	N	367	GLU	2.2
2	P	334	ARG	2.2
2	P	424	ASN	2.2
2	P	566	SER	2.2
2	P	333	ILE	2.1
2	O	125	GLU	2.1
2	N	486[A]	LYS	2.1
2	O	398	ASP	2.1
2	O	233	THR	2.1
1	A	356	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	631	LEU	2.1
1	B	500	CYS	2.1
1	D	470	CYS	2.1
2	P	336	GLY	2.1
2	P	692	GLY	2.1
2	P	13	PRO	2.1
2	O	432	LYS	2.1
2	P	569	ASP	2.1
2	M	318	LEU	2.1
1	C	551	VAL	2.1
2	O	370	GLY	2.1
2	O	670	MET	2.1
1	C	498	THR	2.1
1	D	42	ASP	2.1
2	P	374	ASP	2.1
1	A	538	GLU	2.1
2	N	14	GLU	2.1
2	O	9	GLU	2.1
2	P	575	SER	2.1
1	D	304	ALA	2.1
2	P	694	ASP	2.1
2	O	464	GLN	2.1
1	B	443	GLN	2.1
1	D	580	ALA	2.1
2	O	455	GLU	2.0
2	N	650	THR	2.0
1	D	412	LYS	2.0
1	A	467	ILE	2.0
1	D	20	MET	2.0
2	P	476	GLU	2.0
1	A	469	GLY	2.0
2	P	682	PHE	2.0
2	O	609	ASN	2.0
1	C	81	THR	2.0
2	O	299	ASP	2.0
2	O	620	GLY	2.0
2	P	353	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	863	6/6	0.66	0.32	47,56,56,58	0
9	NA	P	730	1/1	0.84	0.10	35,35,35,35	0
9	NA	O	730	1/1	0.86	0.06	70,70,70,70	0
5	GOL	D	863	6/6	0.89	0.14	43,46,48,48	0
5	GOL	A	863	6/6	0.92	0.13	26,30,33,37	0
8	ACT	P	953	3/4	0.92	0.26	53,53,54,54	0
8	ACT	N	953	3/4	0.93	0.17	59,59,59,59	0
8	ACT	O	953	3/4	0.93	0.30	100,100,100,100	0
3	SF4	O	900	8/8	0.94	0.07	61,63,67,67	0
8	ACT	M	953	3/4	0.96	0.13	44,44,44,45	0
7	NI	O	951	1/1	0.96	0.04	76,76,76,76	0
5	GOL	B	863	6/6	0.96	0.09	26,30,34,37	0
6	CU1	O	950	1/1	0.97	0.06	82,82,82,82	0
3	SF4	P	900	8/8	0.98	0.07	40,40,41,46	0
9	NA	M	730	1/1	0.98	0.09	29,29,29,29	0
6	CU1	P	950	1/1	0.98	0.05	55,55,55,55	0
3	SF4	C	700	8/8	0.98	0.09	28,32,35,35	0
4	XCC	C	800	9/9	0.98	0.13	25,27,34,35	0
9	NA	N	730	1/1	0.98	0.07	28,28,28,28	0
3	SF4	M	900	8/8	0.99	0.09	22,25,26,28	0
6	CU1	N	950	1/1	0.99	0.05	38,38,38,38	0
3	SF4	C	750	8/8	0.99	0.09	28,30,31,32	0
3	SF4	A	750	8/8	0.99	0.11	14,17,17,18	0
6	CU1	M	950	1/1	0.99	0.07	43,43,43,43	0
4	XCC	D	800	9/9	0.99	0.13	33,35,41,45	0
4	XCC	A	800	9/9	0.99	0.12	20,24,29,30	0
7	NI	P	951	1/1	0.99	0.04	39,39,39,39	0
3	SF4	B	750	8/8	0.99	0.11	17,18,18,19	0
3	SF4	A	700	8/8	0.99	0.08	17,19,20,22	0
4	XCC	B	800	9/9	0.99	0.12	16,20,25,27	0
3	SF4	D	750	8/8	0.99	0.12	26,28,29,29	0
3	SF4	N	900	8/8	0.99	0.09	25,26,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NI	N	951	1/1	1.00	0.08	29,29,29,29	0
7	NI	M	951	1/1	1.00	0.07	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.