



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:47 am BST

PDB ID : 3I04  
Title : Cyanide-bound structure of bifunctional carbon monoxide dehydrogenase/acyl-CoA synthase from Moorella thermoacetica, cyanide-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

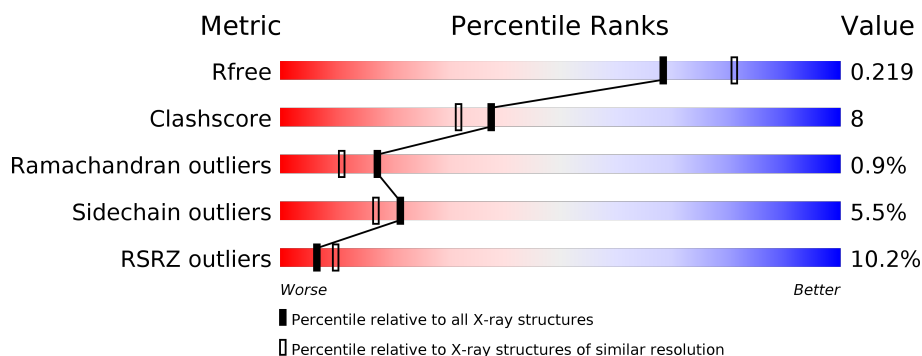
# 1 Overall quality at a glance

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	673	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> <div>.</div> </div>
1	B	673	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> <div>.</div> </div>
1	C	673	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	D	673	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> <div>.</div> </div>
2	M	728	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>11%</div> </div> <div>.</div> </div>
2	N	728	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>11%</div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	O	728	
2	P	728	

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
5	CYN	A	900	-	-	X	-
5	CYN	C	900	-	-	X	-
6	GOL	C	963	-	-	X	-
6	GOL	D	963	-	-	X	-
9	ACT	N	953	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 45801 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.

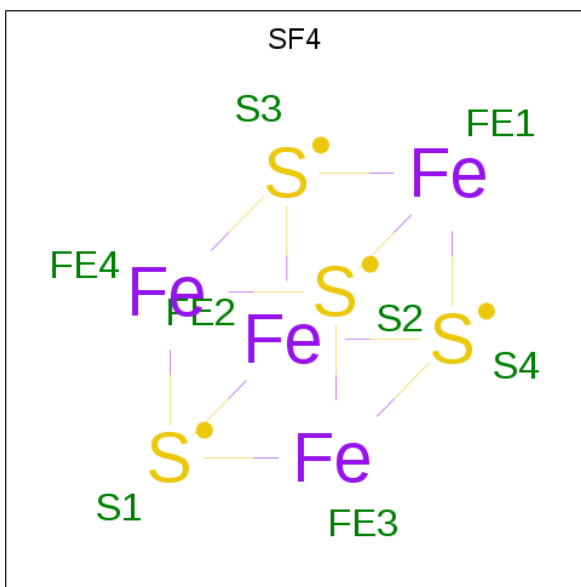
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	5	0
			5134	3226	900	965	43			
1	B	673	Total	C	N	O	S	0	7	0
			5134	3227	895	969	43			
1	C	673	Total	C	N	O	S	0	3	0
			5103	3208	888	965	42			
1	D	673	Total	C	N	O	S	0	0	0
			5088	3199	888	959	42			

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

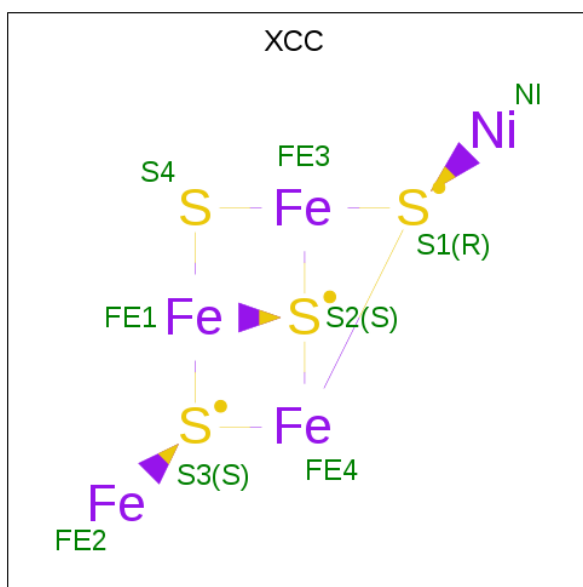
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5766	3695	962	1074	35			
2	N	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	O	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	P	728	Total	C	N	O	S	0	2	0
			5757	3690	963	1069	35			

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



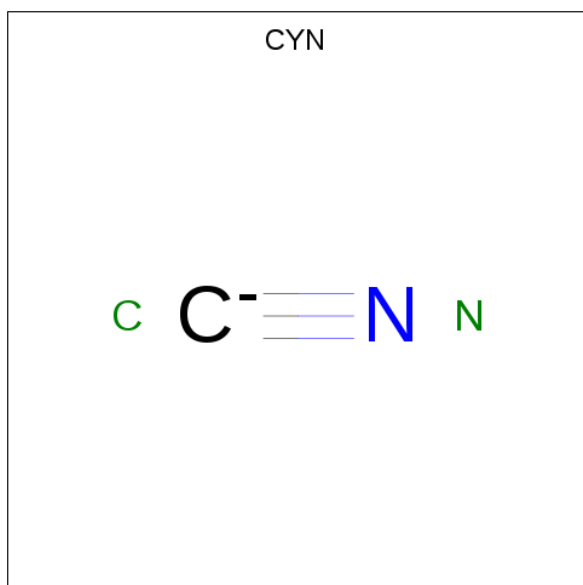
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3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



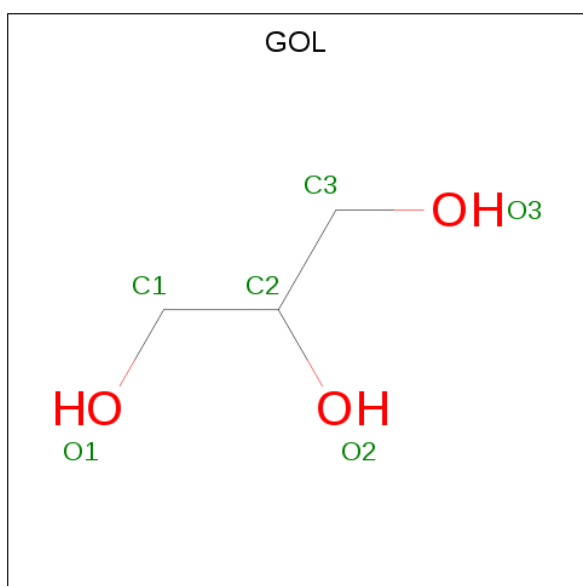
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is CYANIDE ION (three-letter code: CYN) (formula: CN).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N 2 1 1	0	0
5	B	1	Total C N 2 1 1	0	0
5	C	1	Total C N 2 1 1	0	0
5	D	1	Total C N 2 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 7 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	P	1	Total Cu 1 1	0	0
7	O	1	Total Cu 1 1	0	0

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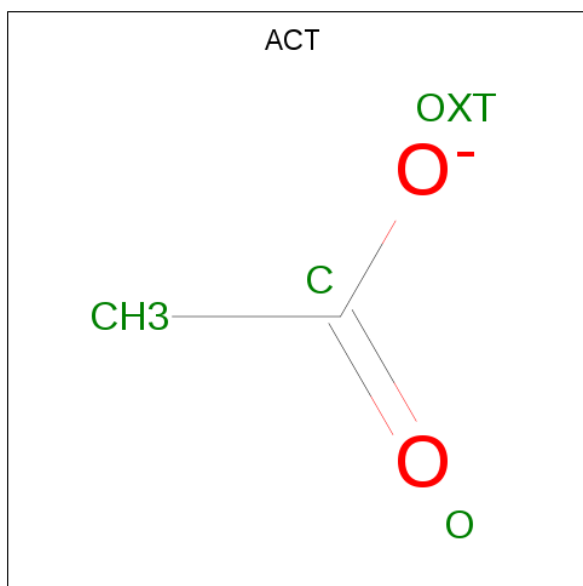
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	N	1	Total	Cu	0	0
			1	1		
7	M	1	Total	Cu	0	0
			1	1		

- Molecule 8 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 9 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
9	M	1	Total	C	O	0	0
			3	2	1		
9	N	1	Total	C	O	0	0
			3	2	1		
9	O	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	P	1	Total	C	O	0	0
			3	2	1		

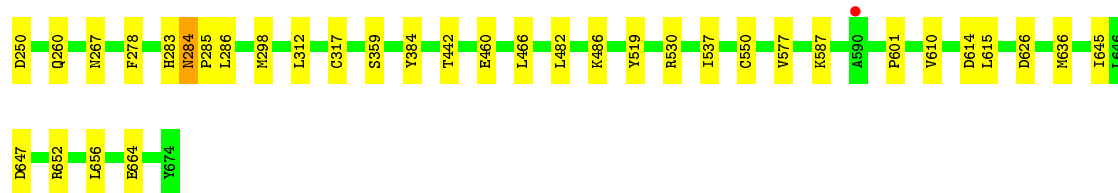
- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

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

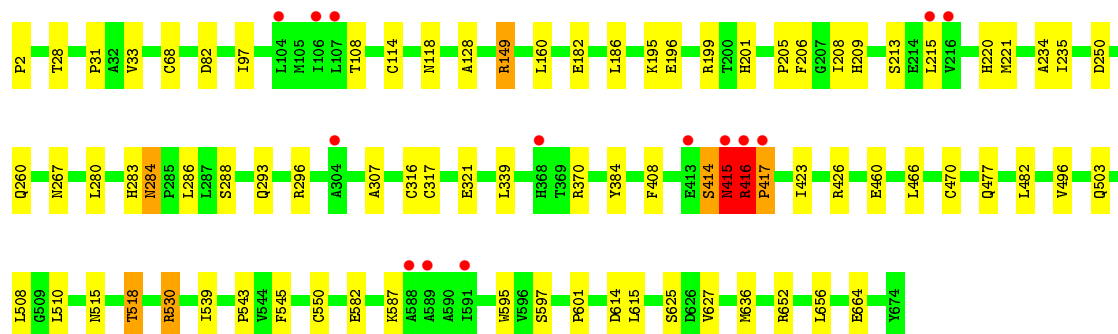
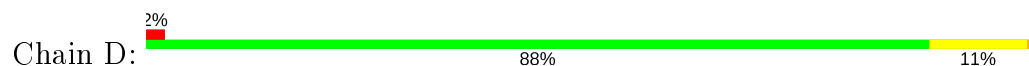
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	306	Total	O	0	0
			306	306		
11	B	375	Total	O	0	0
			375	375		
11	C	275	Total	O	0	0
			275	275		
11	D	240	Total	O	0	0
			240	240		
11	M	326	Total	O	0	0
			326	326		
11	N	337	Total	O	0	0
			337	337		
11	O	83	Total	O	0	0
			83	83		
11	P	213	Total	O	0	0
			213	213		

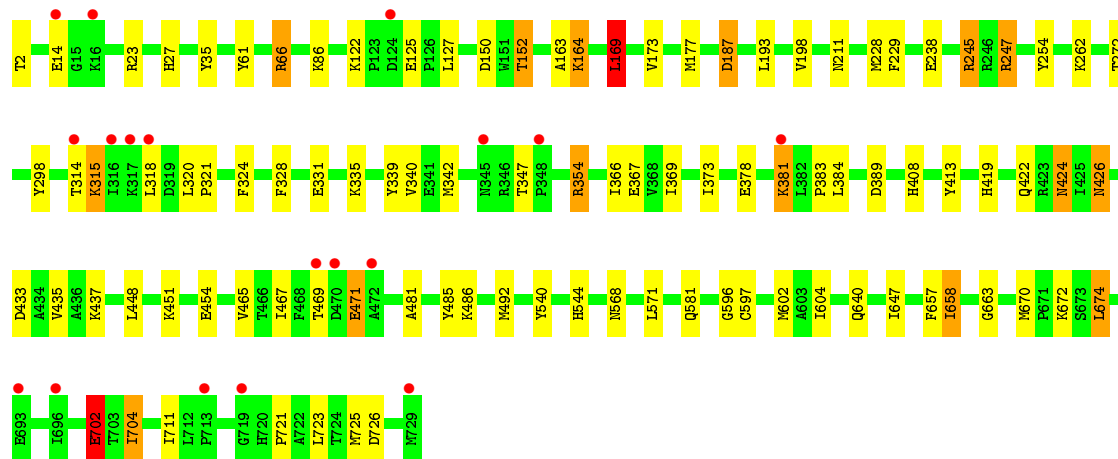
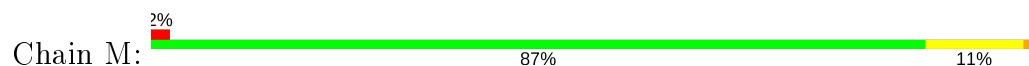




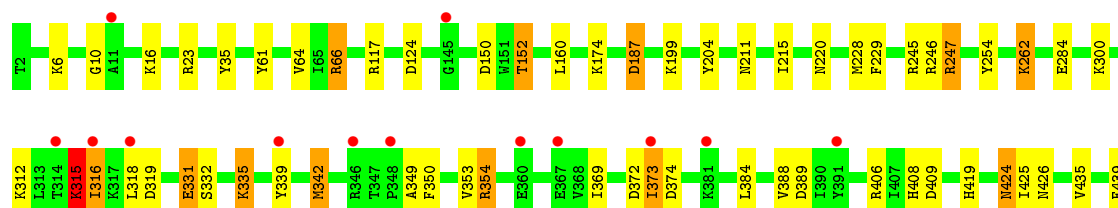
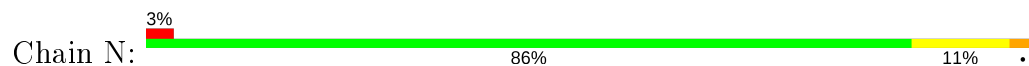
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

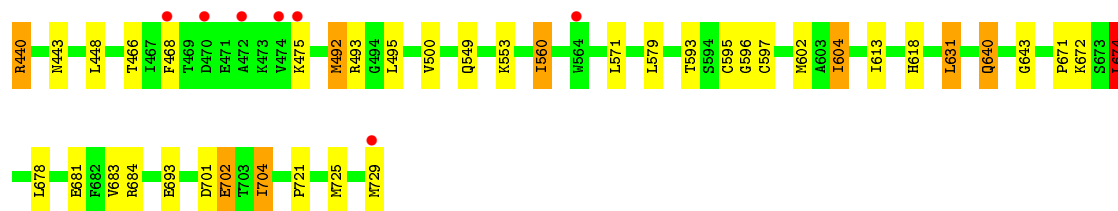


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

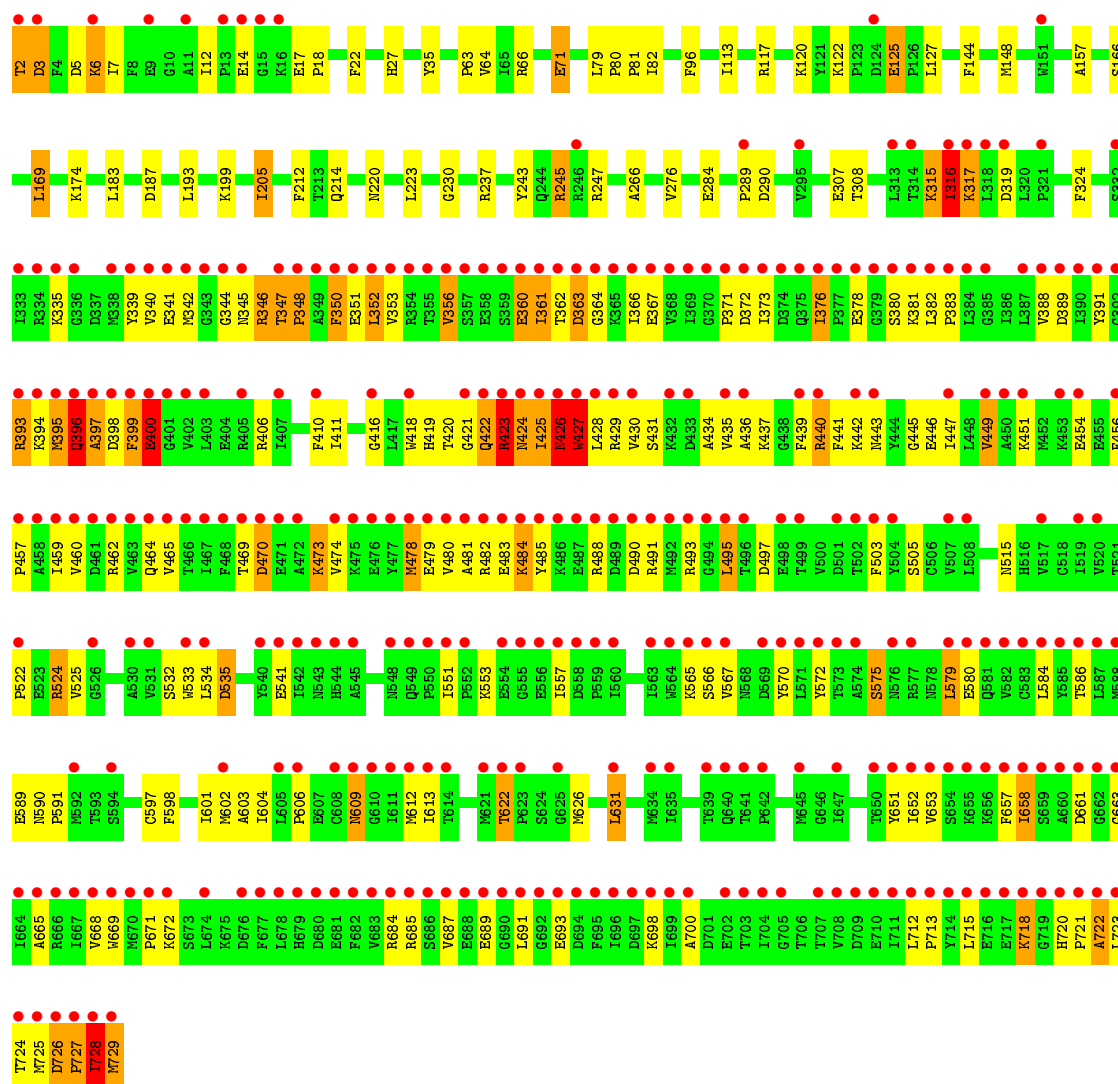
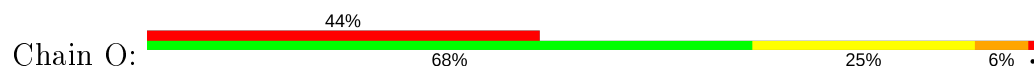


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

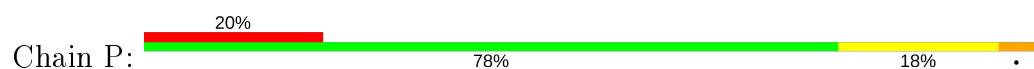


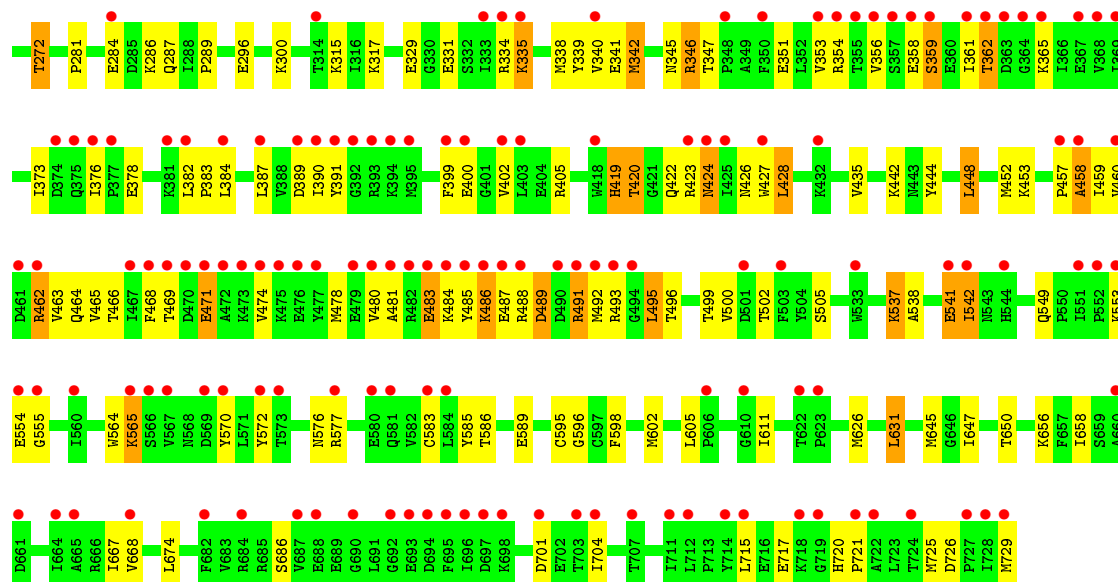


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



• 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, $\alpha$ , $\beta$ , $\gamma$	99.83Å 136.77Å 141.61Å 101.23° 109.18° 103.87°	Depositor
Resolution (Å)	48.39 – 2.15 48.40 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.39-2.15) 96.5 (48.40-2.15)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.31 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.172 , 0.221 0.172 , 0.219	Depositor DCC
$R_{free}$ test set	17112 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	45801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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, CYN

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	0.97	2/5230 (0.0%)	0.82	3/7086 (0.0%)
1	B	0.99	2/5244 (0.0%)	0.82	1/7105 (0.0%)
1	C	0.92	1/5200 (0.0%)	0.81	1/7048 (0.0%)
1	D	0.88	1/5181 (0.0%)	0.80	3/7021 (0.0%)
2	M	0.89	1/5909 (0.0%)	0.81	3/8000 (0.0%)
2	N	0.88	0/5885	0.80	3/7968 (0.0%)
2	O	0.76	0/5885	0.79	3/7968 (0.0%)
2	P	0.76	0/5896	0.75	2/7982 (0.0%)
All	All	0.88	7/44430 (0.0%)	0.80	19/60178 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	GLY	CA-C	-5.65	1.42	1.51
1	D	414	SER	C-O	-5.59	1.12	1.23
1	C	214	GLU	CG-CD	5.53	1.60	1.51
1	B	204	VAL	CB-CG1	5.34	1.64	1.52
1	A	564	ALA	CA-CB	5.25	1.63	1.52
2	M	702	GLU	CG-CD	-5.12	1.44	1.51
1	B	321	GLU	CG-CD	5.03	1.59	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	428	LEU	CA-CB-CG	5.72	128.46	115.30
2	M	198	VAL	CG1-CB-CG2	5.67	119.98	110.90
2	O	237	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	N	631	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	149	ARG	NE-CZ-NH1	5.56	123.08	120.30
2	O	400	GLU	N-CA-C	-5.56	95.99	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	ARG	C-N-CD	-5.41	108.71	120.60
1	C	12	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	M	597	CYS	CA-CB-SG	-5.39	104.30	114.00
2	N	597	CYS	CA-CB-SG	-5.36	104.36	114.00
2	O	423	ARG	NE-CZ-NH2	-5.31	117.64	120.30
2	N	674	LEU	CB-CG-CD2	5.29	119.99	111.00
1	A	139	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	149	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	176	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	87	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	376	ASP	CB-CG-OD1	5.11	122.90	118.30
2	P	420	THR	N-CA-C	-5.11	97.20	111.00
2	M	169	LEU	CB-CG-CD2	5.03	119.54	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5134	0	5139	59	0
1	B	5134	0	5133	64	0
1	C	5103	0	5090	47	0
1	D	5088	0	5086	61	0
2	M	5766	0	5723	59	0
2	N	5746	0	5710	61	0
2	O	5746	0	5711	228	0
2	P	5757	0	5722	124	0
3	A	16	0	0	0	0
3	B	8	0	0	0	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	0	0
3	O	8	0	0	0	0
3	P	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
5	A	2	0	0	2	0
5	B	2	0	0	0	0
5	C	2	0	0	3	0
5	D	2	0	0	1	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
6	C	6	0	8	4	0
6	D	6	0	8	6	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	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	M	3	0	3	1	0
9	N	3	0	3	3	0
9	O	3	0	3	1	0
9	P	3	0	3	1	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
11	A	306	0	0	5	0
11	B	375	0	0	5	0
11	C	275	0	0	5	0
11	D	240	0	0	5	0
11	M	326	0	0	4	0
11	N	337	0	0	9	0
11	O	83	0	0	1	0
11	P	213	0	0	3	0
All	All	45801	0	43358	673	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 8.

All (673) 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:370:ARG:HD2	11:B:1495:HOH:O	1.33	1.28
2:O:425:ILE:HD12	2:O:426:ASN:N	1.48	1.28
2:O:395:MET:SD	2:O:399:PHE:HE2	1.57	1.27
2:O:425:ILE:HD12	2:O:425:ILE:C	1.47	1.27
1:A:105:MET:CE	1:B:72:MET:HG3	1.69	1.23
1:A:105:MET:HE1	1:B:72:MET:CG	1.74	1.17
2:O:425:ILE:O	2:O:426:ASN:ND2	1.81	1.14
2:O:482:ARG:HD2	2:O:485:TYR:OH	1.44	1.13
2:O:490:ASP:O	2:O:493:ARG:HG2	1.48	1.10
2:O:478:MET:HA	2:O:478:MET:HE3	1.13	1.09
1:D:416:ARG:CB	1:D:417:PRO:HD2	1.81	1.08
2:O:395:MET:SD	2:O:399:PHE:CE2	2.48	1.07
2:O:482:ARG:HA	2:O:485:TYR:CE2	1.90	1.06
2:P:338:MET:CE	2:P:341:GLU:HB2	1.86	1.06
2:O:346:ARG:NH2	2:O:427:TRP:CZ2	2.23	1.06
2:P:338:MET:HE1	2:P:341:GLU:HB2	1.34	1.05
2:O:728:ILE:O	2:O:728:ILE:HG23	1.56	1.05
2:M:602:MET:HE3	2:M:647:ILE:HG21	1.37	1.04
2:O:424:ASN:O	2:O:425:ILE:HG22	1.57	1.04
2:O:395:MET:HA	2:O:399:PHE:CZ	1.93	1.03
2:P:391:TYR:HB3	2:P:462:ARG:NH1	1.74	1.03
2:O:657:PHE:CE1	2:O:658:ILE:HD12	1.95	1.02
2:O:426:ASN:O	2:O:427:TRP:HB2	1.19	1.01
2:O:426:ASN:O	2:O:427:TRP:CB	2.05	1.00
2:P:354:ARG:HD2	2:P:356:VAL:HG13	1.44	1.00
2:P:400:GLU:OE2	2:P:484:LYS:HE3	1.62	0.99
1:D:416:ARG:CB	1:D:417:PRO:CD	2.38	0.98
2:O:425:ILE:C	2:O:426:ASN:ND2	2.17	0.96
1:D:114:CYS:HB2	11:D:1014:HOH:O	1.66	0.95
2:O:346:ARG:NH1	2:O:427:TRP:CZ2	2.36	0.94
2:O:622:THR:HG23	2:O:626:MET:O	1.68	0.92
2:O:482:ARG:HD2	2:O:485:TYR:HH	1.33	0.91
2:O:395:MET:HA	2:O:399:PHE:CE2	2.06	0.91
2:P:362:THR:H	2:P:464:GLN:HE21	1.18	0.91
2:O:425:ILE:CD1	2:O:426:ASN:N	2.34	0.89
2:O:478:MET:CE	2:O:478:MET:HA	2.00	0.88
1:A:105:MET:HE1	1:B:72:MET:HG3	0.90	0.87
2:O:478:MET:CA	2:O:478:MET:HE3	2.00	0.87
2:P:400:GLU:OE2	2:P:484:LYS:CE	2.23	0.87
1:C:114:CYS:HB2	11:C:1383:HOH:O	1.74	0.86
2:O:316:ILE:CG2	2:O:454:GLU:HG3	2.07	0.84
2:O:346:ARG:HH22	2:O:427:TRP:HZ2	1.23	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:482:ARG:HA	2:O:485:TYR:CZ	2.13	0.84
2:O:481:ALA:O	2:O:485:TYR:CD2	2.31	0.83
2:P:483:GLU:OE2	2:P:483:GLU:HA	1.77	0.83
2:O:346:ARG:NH2	2:O:427:TRP:CH2	2.43	0.82
1:C:122:HIS:HD2	11:C:905:HOH:O	1.60	0.82
2:P:354:ARG:HD2	2:P:356:VAL:CG1	2.11	0.81
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.63	0.80
2:O:425:ILE:O	2:O:426:ASN:CB	2.24	0.80
2:P:602:MET:HE3	2:P:645:MET:HE2	1.63	0.80
2:O:728:ILE:O	2:O:728:ILE:CG2	2.30	0.80
2:O:346:ARG:CZ	2:O:427:TRP:CZ2	2.64	0.79
2:P:424:ASN:H	2:P:424:ASN:HD22	1.30	0.79
2:O:490:ASP:O	2:O:493:ARG:CG	2.30	0.79
2:N:229:PHE:CD1	9:N:953:ACT:H2	2.18	0.79
1:D:182:GLU:OE2	1:D:199:ARG:HD3	1.81	0.78
1:C:614:ASP:H	6:C:963:GOL:H11	1.49	0.78
1:C:550:CYS:HB3	5:C:900:CYN:N	1.99	0.78
2:O:376:ILE:HD12	2:O:382:LEU:HD21	1.63	0.77
2:O:424:ASN:O	2:O:425:ILE:CG2	2.30	0.77
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.20	0.77
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.50	0.77
2:O:12:ILE:HG21	2:O:17:GLU:HG3	1.67	0.76
2:O:482:ARG:CD	2:O:485:TYR:OH	2.30	0.76
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.67	0.76
2:O:481:ALA:O	2:O:485:TYR:CE2	2.39	0.75
2:O:346:ARG:NH2	2:O:427:TRP:HZ2	1.79	0.75
2:M:335:LYS:HD2	2:M:335:LYS:H	1.52	0.74
2:O:376:ILE:CD1	2:O:382:LEU:HD21	2.17	0.74
2:M:602:MET:HE2	2:M:657:PHE:HE2	1.51	0.74
2:O:651:TYR:CD2	2:O:657:PHE:CD2	2.76	0.74
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.00	0.74
2:N:354:ARG:HD2	2:N:389:ASP:OD2	1.86	0.74
2:P:602:MET:HE3	2:P:645:MET:CE	2.17	0.74
2:O:726:ASP:OD2	2:O:729:MET:HB2	1.87	0.74
1:C:550:CYS:CB	5:C:900:CYN:N	2.51	0.73
2:M:433:ASP:OD1	2:M:437:LYS:HE2	1.89	0.73
2:O:425:ILE:HD12	2:O:426:ASN:CA	2.18	0.72
2:P:346:ARG:HH11	2:P:346:ARG:HB2	1.55	0.72
2:N:549:GLN:HG2	11:N:2291:HOH:O	1.89	0.72
2:N:424:ASN:HD22	2:N:424:ASN:H	1.38	0.72
2:O:356:VAL:HG23	2:O:361:ILE:HD11	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:657:PHE:CE1	2:O:658:ILE:CD1	2.70	0.72
2:O:352:LEU:CD2	2:O:484:LYS:HG3	2.19	0.72
1:C:260:GLN:NE2	11:C:785:HOH:O	2.23	0.71
2:O:352:LEU:HD13	2:O:481:ALA:HA	1.71	0.71
2:O:424:ASN:C	2:O:425:ILE:CG2	2.59	0.71
2:N:701:ASP:H	2:N:704:ILE:HG23	1.54	0.71
2:O:651:TYR:CE2	2:O:657:PHE:CD2	2.79	0.71
2:P:400:GLU:CD	2:P:484:LYS:HE3	2.12	0.71
2:P:362:THR:H	2:P:464:GLN:NE2	1.88	0.70
2:P:491:ARG:O	2:P:495:LEU:HB2	1.90	0.70
2:O:418:TRP:O	2:O:428:LEU:HA	1.91	0.70
2:P:423:ARG:HH21	2:P:488:ARG:NH1	1.88	0.70
2:O:396:GLN:HE22	2:O:398:ASP:HB2	1.56	0.70
2:P:424:ASN:N	2:P:424:ASN:HD22	1.90	0.70
2:O:399:PHE:O	2:O:399:PHE:CD2	2.44	0.70
2:M:408:HIS:HD2	2:M:419:HIS:ND1	1.90	0.70
2:P:356:VAL:O	2:P:391:TYR:HB2	1.91	0.70
1:B:535:ALA:HB3	1:B:537:ILE:HG12	1.74	0.70
2:M:150:ASP:OD2	2:M:152:THR:HG23	1.92	0.70
2:P:338:MET:HE1	2:P:341:GLU:CB	2.17	0.70
2:O:665:ALA:HB2	2:O:691:LEU:HD11	1.74	0.70
1:D:614:ASP:N	6:D:963:GOL:H11	2.06	0.70
2:N:335:LYS:HD3	2:N:335:LYS:N	2.05	0.70
2:O:315:LYS:HD3	2:O:317:LYS:HE2	1.74	0.69
6:C:963:GOL:H12	2:O:27:HIS:CE1	2.28	0.69
2:N:369:ILE:HD12	2:N:466:THR:CG2	2.23	0.69
2:O:395:MET:CA	2:O:399:PHE:CZ	2.75	0.69
2:O:410:PHE:CD1	2:O:451:LYS:HD3	2.28	0.69
1:C:587:LYS:H	1:D:220:HIS:HE1	1.42	0.68
1:C:614:ASP:N	6:C:963:GOL:H11	2.08	0.68
1:D:515:ASN:HD22	1:D:518:THR:HG21	1.57	0.68
2:O:316:ILE:HG21	2:O:454:GLU:HG3	1.76	0.68
1:D:482:LEU:HD11	1:D:508:LEU:HD13	1.75	0.68
2:O:425:ILE:O	2:O:426:ASN:CG	2.31	0.68
2:P:150:ASP:OD2	2:P:152:THR:HG22	1.94	0.68
1:B:114[B]:CYS:SG	1:B:208:ILE:HG21	2.34	0.68
2:O:423:ARG:HB3	2:O:424:ASN:HD22	1.58	0.68
2:O:418:TRP:HE3	2:O:429:ARG:HD2	1.59	0.68
2:O:445:GLY:O	2:O:449:VAL:HG23	1.94	0.68
1:A:284:ASN:HD22	1:A:286:LEU:H	1.42	0.67
2:M:704:ILE:HD11	2:M:711:ILE:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:651:TYR:CD2	2:O:657:PHE:HD2	2.12	0.67
1:A:114[B]:CYS:SG	1:A:208:ILE:HG21	2.34	0.67
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.58	0.67
2:O:658:ILE:O	2:O:658:ILE:HG22	1.95	0.67
2:P:500:VAL:O	2:P:553:LYS:NZ	2.23	0.67
2:O:485:TYR:HA	2:O:488:ARG:HE	1.58	0.67
2:N:150:ASP:OD2	2:N:152:THR:CG2	2.42	0.67
2:O:653:VAL:O	2:O:685:ARG:HD2	1.94	0.67
2:P:353:VAL:O	2:P:400:GLU:HG3	1.95	0.67
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.25	0.67
2:O:524:ARG:HG3	2:O:524:ARG:O	1.94	0.66
1:B:482:LEU:HD12	1:B:486:LYS:HE3	1.77	0.66
2:M:424:ASN:H	2:M:424:ASN:HD22	1.41	0.66
2:O:363:ASP:HB2	2:O:462:ARG:HD2	1.76	0.66
2:O:422:GLN:O	2:O:423:ARG:HB2	1.94	0.66
1:C:220:HIS:HE1	1:D:587:LYS:H	1.42	0.65
2:P:424:ASN:ND2	2:P:424:ASN:H	1.93	0.65
1:A:149[B]:ARG:NH2	1:A:250:ASP:OD2	2.29	0.65
1:B:370:ARG:HB3	11:B:1495:HOH:O	1.96	0.65
1:A:220:HIS:HD2	1:A:221:MET:O	1.80	0.65
2:P:246:ARG:HG2	2:P:246:ARG:HH11	1.60	0.65
2:O:482:ARG:CA	2:O:485:TYR:CE2	2.75	0.65
1:B:114[A]:CYS:SG	1:B:209:HIS:NE2	2.70	0.64
2:O:340:VAL:HG21	2:O:441:PHE:HZ	1.62	0.64
2:O:726:ASP:O	2:O:727:PRO:C	2.33	0.64
2:N:406:ARG:NH1	2:N:409:ASP:OD2	2.30	0.64
1:B:296:ARG:NH1	11:B:1789:HOH:O	2.31	0.64
1:A:220:HIS:HE1	1:B:587:LYS:H	1.46	0.64
2:O:420:THR:O	2:O:426:ASN:HA	1.98	0.64
2:O:424:ASN:N	2:O:424:ASN:HD22	1.96	0.64
1:C:284:ASN:C	1:C:284:ASN:HD22	2.02	0.63
1:A:105:MET:CE	1:B:72:MET:CG	2.51	0.63
2:M:451:LYS:NZ	2:M:454:GLU:OE2	2.25	0.63
2:O:604:ILE:HD12	2:O:606:PRO:HD3	1.79	0.63
2:O:551:ILE:HD13	2:O:567:VAL:HG23	1.81	0.63
1:A:299:GLU:O	1:A:303:LYS:HG2	1.98	0.62
2:O:376:ILE:HD12	2:O:382:LEU:CD2	2.29	0.62
2:P:402:VAL:HG21	2:P:538:ALA:HB2	1.82	0.62
2:P:483:GLU:O	2:P:487:GLU:CB	2.48	0.62
2:O:572:TYR:HD1	2:O:580:GLU:HB3	1.63	0.62
2:P:341:GLU:CD	2:P:427:TRP:HE1	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HH11	1:A:370:ARG:HG2	1.64	0.62
2:N:335:LYS:HD3	2:N:335:LYS:H	1.64	0.62
2:M:721:PRO:O	2:M:725:MET:HG3	2.00	0.62
1:A:209:HIS:HD2	1:B:213:SER:OG	1.83	0.62
2:P:537:LYS:HD3	2:P:541:GLU:OE2	1.99	0.61
2:O:470:ASP:HB3	2:O:473:LYS:HB3	1.81	0.61
2:O:430:VAL:HG12	2:O:434:ALA:HB3	1.82	0.61
1:D:515:ASN:HD22	1:D:518:THR:CG2	2.13	0.61
2:O:352:LEU:HD21	2:O:484:LYS:HG3	1.81	0.61
2:P:341:GLU:OE2	2:P:346:ARG:NH1	2.34	0.60
2:O:144:PHE:O	2:O:148:MET:HG3	2.01	0.60
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.37	0.60
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.34	0.60
1:C:220:HIS:HD2	1:C:221:MET:O	1.84	0.60
2:O:727:PRO:O	2:O:729:MET:N	2.35	0.60
1:D:284:ASN:HD22	1:D:286:LEU:H	1.50	0.60
2:M:367:GLU:HG3	2:M:369:ILE:HD11	1.84	0.60
2:O:490:ASP:C	2:O:493:ARG:HG2	2.21	0.60
2:N:150:ASP:OD2	2:N:152:THR:HG23	2.02	0.60
2:O:478:MET:HE2	2:O:478:MET:O	2.02	0.60
1:C:284:ASN:HD22	1:C:286:LEU:H	1.50	0.60
2:O:430:VAL:HG21	2:O:439:PHE:CE2	2.37	0.60
2:P:419:HIS:ND1	2:P:420:THR:N	2.49	0.60
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.37	0.60
2:O:341:GLU:CG	2:O:427:TRP:HE1	2.14	0.59
2:O:651:TYR:CD2	2:O:657:PHE:CE2	2.91	0.59
2:P:334:ARG:HG2	11:P:1790:HOH:O	2.03	0.59
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.85	0.59
2:N:354:ARG:CD	2:N:389:ASP:OD2	2.50	0.59
2:P:300:LYS:NZ	11:P:1581:HOH:O	2.34	0.59
2:N:117[A]:ARG:HG3	11:N:2259:HOH:O	2.01	0.59
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.83	0.59
1:C:196[B]:GLU:OE2	2:O:120:LYS:NZ	2.36	0.59
2:P:483:GLU:O	2:P:487:GLU:HB2	2.03	0.59
1:D:195:LYS:O	1:D:199:ARG:HG3	2.03	0.59
1:D:466:LEU:HD22	1:D:595:TRP:HZ2	1.68	0.59
2:N:229:PHE:HD1	9:N:953:ACT:H2	1.66	0.59
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.33	0.58
1:B:442:THR:HG21	1:B:535:ALA:HA	1.83	0.58
2:M:602:MET:HE2	2:M:657:PHE:CE2	2.34	0.58
1:A:119:HIS:HE1	11:A:1427:HOH:O	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:245:ARG:HD3	11:M:918:HOH:O	2.02	0.58
2:N:595:CYS:HB2	9:N:953:ACT:H1	1.84	0.58
2:O:425:ILE:C	2:O:426:ASN:CG	2.55	0.58
2:O:346:ARG:NH1	2:O:427:TRP:CE2	2.65	0.58
2:O:18:PRO:HD2	2:O:22:PHE:CZ	2.38	0.58
2:O:425:ILE:O	2:O:426:ASN:HB3	2.01	0.58
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.66	0.58
1:B:114[A]:CYS:SG	1:B:209:HIS:CD2	2.97	0.58
2:O:491:ARG:O	2:O:495:LEU:HB2	2.03	0.58
2:O:371:PRO:HD2	2:O:469:THR:HB	1.84	0.58
2:P:361:ILE:HG21	2:P:462:ARG:HD3	1.85	0.58
1:A:587:LYS:H	1:B:220:HIS:HE1	1.52	0.57
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.39	0.57
2:O:324:PHE:CE2	2:O:451:LYS:HE2	2.39	0.57
1:D:614:ASP:H	6:D:963:GOL:H11	1.68	0.57
2:O:346:ARG:HG3	2:O:381:LYS:NZ	2.19	0.57
2:O:394:LYS:HG2	2:O:395:MET:H	1.68	0.57
2:O:658:ILE:CG2	2:O:661:ASP:HB2	2.33	0.57
1:A:114[B]:CYS:SG	1:A:208:ILE:CG2	2.93	0.57
1:C:209:HIS:HD2	1:D:213:SER:OG	1.87	0.57
2:O:352:LEU:HD22	2:O:484:LYS:HG3	1.84	0.57
2:M:602:MET:CE	2:M:647:ILE:HD13	2.34	0.57
2:O:722:ALA:HA	2:O:725:MET:SD	2.44	0.57
2:P:583:CYS:HB2	2:P:586:THR:HG22	1.87	0.57
2:O:64:VAL:HB	2:O:223:LEU:HD12	1.87	0.57
1:A:426:ARG:HH21	1:A:539:ILE:HD12	1.70	0.57
2:N:23:ARG:NH1	11:N:855:HOH:O	2.36	0.57
2:O:424:ASN:N	2:O:424:ASN:ND2	2.50	0.57
2:P:402:VAL:HG21	2:P:538:ALA:CB	2.35	0.57
2:O:316:ILE:HG23	2:O:454:GLU:HG3	1.86	0.57
1:D:414:SER:O	1:D:415:ASN:C	2.40	0.56
2:P:399:PHE:HE2	2:P:541:GLU:HG3	1.70	0.56
1:A:577:VAL:HG11	1:A:645:ILE:HG23	1.88	0.56
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.35	0.56
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.40	0.56
2:O:356:VAL:HG23	2:O:361:ILE:CD1	2.36	0.56
2:O:424:ASN:C	2:O:425:ILE:HG23	2.25	0.56
1:B:24:ASN:O	1:B:27:ARG:HG2	2.06	0.56
1:B:482:LEU:CD1	1:B:486:LYS:HE3	2.35	0.55
2:M:383:PRO:HG3	2:M:471:GLU:HG3	1.87	0.55
2:P:457:PRO:O	2:P:458:ALA:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASN:HD22	1:B:450:ARG:HB2	1.72	0.55
2:N:150:ASP:OD2	2:N:152:THR:HG22	2.06	0.55
2:P:602:MET:CE	2:P:647:ILE:HG21	2.36	0.55
1:A:426:ARG:CZ	11:A:2027:HOH:O	2.54	0.55
2:N:335:LYS:H	2:N:335:LYS:CD	2.19	0.55
1:D:426:ARG:NH1	11:D:2194:HOH:O	2.38	0.55
1:D:220:HIS:HD2	1:D:221:MET:O	1.90	0.55
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.07	0.55
2:O:418:TRP:O	2:O:428:LEU:HD13	2.06	0.55
2:M:163:ALA:HB2	2:M:169:LEU:HG	1.89	0.54
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.72	0.54
1:B:537:ILE:CG2	1:B:540:GLY:H	2.20	0.54
2:P:150:ASP:OD2	2:P:152:THR:CG2	2.54	0.54
1:A:368:HIS:NE2	1:A:416:ARG:HG3	2.23	0.54
1:A:122:HIS:HD2	11:A:926:HOH:O	1.90	0.54
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.36	0.54
2:O:480:VAL:O	2:O:484:LYS:HB2	2.07	0.54
2:M:602:MET:CE	2:M:657:PHE:CE2	2.91	0.54
2:N:369:ILE:HD12	2:N:466:THR:HG21	1.89	0.54
2:O:447:ILE:O	2:O:451:LYS:HB2	2.07	0.54
1:C:284:ASN:ND2	1:C:286:LEU:H	2.06	0.54
2:P:420:THR:O	2:P:420:THR:CG2	2.55	0.54
2:N:408:HIS:HD2	2:N:419:HIS:ND1	2.06	0.54
2:O:435:VAL:C	2:O:437:LYS:H	2.10	0.54
2:O:479:GLU:O	2:O:483:GLU:HG3	2.07	0.54
1:A:119:HIS:CE1	11:A:1427:HOH:O	2.60	0.54
2:O:388:VAL:HG13	2:O:465:VAL:HG22	1.88	0.54
2:P:335:LYS:HD2	2:P:335:LYS:H	1.72	0.54
2:N:66:ARG:HD3	11:N:754:HOH:O	2.07	0.53
2:O:157:ALA:HB3	2:O:183:LEU:HD23	1.91	0.53
2:O:425:ILE:C	2:O:426:ASN:HD22	1.88	0.53
2:O:609:ASN:ND2	2:O:725:MET:O	2.41	0.53
2:O:684:ARG:NH1	2:O:685:ARG:HG2	2.23	0.53
1:B:114[B]:CYS:SG	1:B:208:ILE:CG2	2.96	0.53
2:O:324:PHE:CZ	2:O:451:LYS:HE2	2.43	0.53
1:D:470:CYS:O	1:D:582:GLU:HB2	2.09	0.53
1:D:260:GLN:NE2	11:D:1371:HOH:O	2.41	0.53
2:O:416:GLY:O	2:O:430:VAL:HA	2.09	0.53
2:P:387:LEU:O	2:P:465:VAL:HA	2.09	0.53
2:P:457:PRO:O	2:P:458:ALA:HB2	2.08	0.53
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114[A]:CYS:SG	1:A:209:HIS:NE2	2.82	0.53
1:C:149:ARG:HD3	11:C:1313:HOH:O	2.09	0.53
1:A:284:ASN:ND2	1:A:286:LEU:H	2.06	0.53
1:D:601:PRO:HD3	1:D:652:ARG:CZ	2.39	0.53
1:D:550:CYS:HB3	5:D:900:CYN:N	2.24	0.52
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.38	0.52
2:N:349:ALA:HA	2:N:384:LEU:O	2.10	0.52
2:N:618:HIS:CE1	2:N:702:GLU:HG2	2.43	0.52
2:N:681:GLU:HG2	2:N:684:ARG:HH21	1.75	0.52
2:P:354:ARG:CD	2:P:356:VAL:HG13	2.31	0.52
1:B:284:ASN:HD22	1:B:286:LEU:H	1.56	0.52
2:P:602:MET:HE1	2:P:647:ILE:HG21	1.90	0.52
1:C:114:CYS:SG	1:C:209:HIS:NE2	2.83	0.52
2:N:199:LYS:HE3	2:N:204:TYR:OH	2.09	0.52
2:O:503:PHE:O	2:O:551:ILE:N	2.28	0.52
2:M:173:VAL:O	2:M:177:MET:HG3	2.10	0.52
2:O:421:GLY:HA3	2:O:425:ILE:HD11	1.91	0.52
2:P:239:GLU:HG2	11:P:2373:HOH:O	2.08	0.52
2:O:651:TYR:O	2:O:657:PHE:CD2	2.63	0.52
2:P:399:PHE:CE2	2:P:541:GLU:HG3	2.44	0.52
2:M:314:THR:O	2:M:315:LYS:C	2.49	0.51
2:O:80:PRO:HB2	2:O:81:PRO:HD3	1.92	0.51
1:A:201:HIS:HE1	2:M:35:TYR:OH	1.94	0.51
2:M:602:MET:CE	2:M:657:PHE:HE2	2.23	0.51
1:C:186:LEU:HD22	1:C:205:PRO:HD2	1.92	0.51
2:P:174:LYS:HE2	2:P:175:GLU:N	2.26	0.51
1:C:81[B]:THR:HG23	1:C:82:ASP:OD2	2.09	0.51
2:M:150:ASP:OD2	2:M:152:THR:CG2	2.57	0.51
2:O:668:VAL:HG12	2:O:720:HIS:CE1	2.46	0.51
2:P:602:MET:CE	2:P:645:MET:HE3	2.41	0.51
1:A:213:SER:OG	1:B:209:HIS:HD2	1.94	0.51
2:M:339:TYR:HD2	2:M:340:VAL:HG22	1.75	0.51
2:O:478:MET:CE	2:O:478:MET:CA	2.72	0.51
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.91	0.51
2:P:61:TYR:HD1	2:P:66:ARG:HD2	1.76	0.51
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.46	0.51
2:P:419:HIS:C	2:P:419:HIS:ND1	2.64	0.51
2:O:590:ASN:N	2:O:591:PRO:HD3	2.25	0.51
1:B:470:CYS:O	1:B:582:GLU:HB2	2.11	0.51
2:O:658:ILE:HG23	2:O:661:ASP:HB2	1.93	0.51
1:A:200:THR:OG1	1:A:201:HIS:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:CYS:O	1:D:321:GLU:HG2	2.11	0.50
2:P:505:SER:HB3	2:P:570:TYR:CE2	2.46	0.50
2:M:2:THR:N	11:M:2199:HOH:O	2.43	0.50
1:C:460:GLU:CD	1:C:530:ARG:HH22	2.15	0.50
2:M:328:PHE:O	2:M:331:GLU:HB2	2.11	0.50
6:A:963:GOL:H11	2:M:27:HIS:CE1	2.47	0.50
2:N:300:LYS:HD2	11:N:1484:HOH:O	2.11	0.50
2:N:640:GLN:HA	11:N:954:HOH:O	2.10	0.50
2:P:339:TYR:CE1	2:P:435:VAL:HG11	2.47	0.50
2:O:397:ALA:HA	2:O:400:GLU:OE1	2.12	0.49
2:O:425:ILE:N	2:O:426:ASN:ND2	2.59	0.49
2:P:124:ASP:OD1	2:P:125:GLU:OE1	2.29	0.49
1:A:515:ASN:ND2	1:A:518:THR:HG21	2.23	0.49
1:B:201:HIS:HE1	2:N:35:TYR:OH	1.95	0.49
1:D:370:ARG:HD2	1:D:384:TYR:CE2	2.47	0.49
2:N:618:HIS:HE1	2:N:702:GLU:HG2	1.76	0.49
2:O:456:PHE:N	2:O:457:PRO:HD3	2.27	0.49
2:O:657:PHE:O	2:O:663:GLY:HA2	2.12	0.49
2:P:420:THR:O	2:P:420:THR:HG23	2.12	0.49
1:A:220:HIS:CD2	1:A:221:MET:O	2.62	0.49
1:D:114:CYS:SG	1:D:209:HIS:NE2	2.86	0.49
2:O:609:ASN:HB3	2:O:722:ALA:O	2.12	0.49
1:B:394:ILE:HG23	1:B:395:GLU:N	2.28	0.49
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.95	0.49
2:O:522:PRO:HD3	2:O:533:TRP:CD1	2.48	0.49
1:C:577:VAL:HG11	1:C:645:ILE:HG23	1.95	0.49
2:O:602:MET:SD	2:O:658:ILE:HD11	2.53	0.49
2:P:602:MET:CE	2:P:645:MET:CE	2.89	0.49
1:B:305:ALA:HB1	1:B:409:LYS:HE3	1.95	0.49
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.28	0.49
2:O:346:ARG:HG3	2:O:381:LYS:HZ3	1.76	0.49
2:O:411:ILE:HD13	2:O:428:LEU:HD11	1.93	0.49
2:O:443:ASN:HA	2:O:446:GLU:OE2	2.12	0.49
2:P:351:GLU:OE2	2:P:426:ASN:ND2	2.46	0.49
2:P:481:ALA:HB1	2:P:485:TYR:CZ	2.48	0.49
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.95	0.49
2:P:585:TYR:CE2	2:P:656:LYS:HD2	2.47	0.49
1:D:201:HIS:HE1	1:D:627:VAL:HG13	1.77	0.48
2:N:374:ASP:HB3	2:N:440:ARG:HH21	1.77	0.48
2:N:61:TYR:HD1	2:N:66:ARG:HD2	1.78	0.48
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:651:TYR:CE2	2:O:657:PHE:HD2	2.28	0.48
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.38	0.48
2:M:568:ASN:HD21	2:M:581:GLN:HE21	1.61	0.48
2:O:425:ILE:O	2:O:425:ILE:HD12	2.02	0.48
1:D:316:CYS:H	1:D:503:GLN:HE22	1.61	0.48
1:D:615:LEU:H	6:D:963:GOL:C1	2.25	0.48
2:O:396:GLN:NE2	2:O:398:ASP:HB2	2.25	0.48
1:A:550:CYS:HB3	5:A:900:CYN:N	2.29	0.48
2:O:423:ARG:C	2:O:424:ASN:ND2	2.67	0.48
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.78	0.48
2:M:540:TYR:O	2:M:544:HIS:HD2	1.96	0.48
2:N:492:MET:HE2	11:N:1937:HOH:O	2.13	0.48
2:M:424:ASN:HD22	2:M:424:ASN:N	2.07	0.48
2:N:315:LYS:HD2	2:N:315:LYS:H	1.77	0.48
2:O:597:CYS:HB3	9:O:953:ACT:H1	1.96	0.48
1:A:201:HIS:CE1	2:M:35:TYR:OH	2.67	0.48
1:A:104[A]:LEU:CD2	1:B:104[A]:LEU:HD22	2.43	0.48
2:O:289:PRO:O	2:O:290:ASP:HB2	2.12	0.48
1:D:201:HIS:CE1	2:P:35:TYR:OH	2.67	0.48
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.96	0.48
2:P:163:ALA:CB	2:P:169:LEU:HB2	2.44	0.48
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.95	0.48
2:N:602:MET:HE2	2:N:602:MET:HB3	1.75	0.48
2:O:372:ASP:O	2:O:376:ILE:HG12	2.13	0.48
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.44	0.47
2:O:350:PHE:CD1	2:O:481:ALA:HB2	2.49	0.47
1:A:284:ASN:HD21	1:A:286:LEU:HG	1.80	0.47
1:D:215:LEU:HD22	1:D:234:ALA:HA	1.96	0.47
2:O:243:TYR:CE2	2:O:247:ARG:HD2	2.49	0.47
1:A:104[A]:LEU:HD22	1:B:104[A]:LEU:CD2	2.45	0.47
1:C:201:HIS:HE1	2:O:35:TYR:OH	1.97	0.47
2:O:389:ASP:HB2	2:O:464:GLN:HB3	1.95	0.47
1:C:149:ARG:NH2	1:C:250:ASP:OD2	2.46	0.47
2:O:698:LYS:HA	2:O:718:LYS:HE2	1.96	0.47
1:D:515:ASN:ND2	1:D:518:THR:HG21	2.25	0.47
2:O:469:THR:O	2:O:470:ASP:HB2	2.15	0.47
2:O:470:ASP:O	2:O:474:VAL:HG22	2.14	0.47
2:O:230:GLY:HA3	2:O:243:TYR:CE2	2.50	0.47
2:P:611:ILE:HD11	2:P:667:ILE:HG12	1.96	0.47
1:D:284:ASN:HD22	1:D:284:ASN:C	2.18	0.47
1:A:284:ASN:C	1:A:284:ASN:HD22	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:2:THR:HA	2:O:5:ASP:OD1	2.14	0.47
1:A:149[A]:ARG:NH2	1:A:250:ASP:OD2	2.44	0.47
1:A:482:LEU:CD1	1:A:486:LYS:HE3	2.45	0.47
2:O:79:LEU:N	2:O:80:PRO:CD	2.78	0.47
2:P:701:ASP:H	2:P:704:ILE:HD13	1.80	0.47
2:P:555:GLY:HA3	2:P:565:LYS:HB3	1.97	0.47
2:O:341:GLU:CD	2:O:427:TRP:HE1	2.18	0.46
2:P:668:VAL:HB	2:P:715:LEU:HD11	1.97	0.46
1:B:267:ASN:O	1:B:270:VAL:HG22	2.15	0.46
2:M:657:PHE:O	2:M:663:GLY:HA2	2.15	0.46
2:O:113:ILE:O	2:O:117[A]:ARG:HG3	2.15	0.46
6:D:963:GOL:H12	2:P:27:HIS:CE1	2.50	0.46
2:P:351:GLU:HG2	2:P:426:ASN:OD1	2.16	0.46
2:O:376:ILE:HD13	2:O:382:LEU:HD21	1.97	0.46
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.80	0.46
2:N:160:LEU:HD13	2:N:215:ILE:HD13	1.97	0.46
2:O:157:ALA:HB3	2:O:183:LEU:HD22	1.98	0.46
2:P:444:TYR:O	2:P:448:LEU:HD22	2.16	0.46
1:A:482:LEU:HD13	1:A:486:LYS:HE3	1.97	0.46
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.51	0.46
2:M:339:TYR:CG	2:M:435:VAL:HG21	2.49	0.46
1:A:483:THR:HB	1:A:638:PRO:HB2	1.97	0.46
1:B:661[A]:GLU:HG3	1:B:665:ARG:HH21	1.81	0.46
2:N:604:ILE:HG13	2:N:643:GLY:O	2.16	0.46
2:O:439:PHE:CE1	2:O:443:ASN:HB2	2.51	0.46
2:P:341:GLU:CD	2:P:427:TRP:NE1	2.69	0.46
2:P:384:LEU:HA	2:P:468:PHE:O	2.16	0.46
2:N:500:VAL:O	2:N:553:LYS:NZ	2.42	0.46
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.97	0.46
1:B:367:TYR:HA	1:B:416:ARG:HH12	1.81	0.46
1:C:118:ASN:OD1	1:C:209:HIS:HE1	1.99	0.46
1:D:201:HIS:CE1	1:D:627:VAL:HG13	2.50	0.46
2:O:566:SER:HB3	11:O:1472:HOH:O	2.16	0.46
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.98	0.46
1:D:201:HIS:HE1	2:P:35:TYR:OH	1.99	0.46
1:C:114:CYS:SG	1:C:209:HIS:CD2	3.09	0.45
2:N:674:LEU:HD22	2:N:678:LEU:HG	1.98	0.45
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.50	0.45
2:M:347:THR:CG2	2:M:381:LYS:HG3	2.47	0.45
2:O:423:ARG:C	2:O:424:ASN:HD22	2.19	0.45
2:O:399:PHE:CZ	2:O:459:ILE:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:481:ALA:O	2:O:485:TYR:HD2	1.90	0.45
1:C:220:HIS:CD2	1:C:221:MET:O	2.67	0.45
1:B:201:HIS:CE1	2:N:35:TYR:OH	2.70	0.45
2:O:339:TYR:HB3	2:O:373:ILE:HD11	1.99	0.45
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.99	0.45
2:P:338:MET:HG2	2:P:339:TYR:H	1.81	0.45
1:B:537:ILE:HG22	1:B:540:GLY:H	1.81	0.45
1:B:539:ILE:H	1:B:539:ILE:HD13	1.81	0.45
1:C:614:ASP:H	6:C:963:GOL:H32	1.81	0.45
2:P:389:ASP:HB2	2:P:464:GLN:HG3	1.99	0.45
2:P:483:GLU:O	2:P:487:GLU:HB3	2.15	0.45
1:A:209:HIS:HD2	1:B:213:SER:CB	2.30	0.45
2:N:342:MET:N	2:N:342:MET:SD	2.90	0.45
2:O:470:ASP:HB3	2:O:473:LYS:CB	2.47	0.45
1:D:466:LEU:CD2	1:D:595:TRP:CZ2	2.97	0.45
2:O:505:SER:HB3	2:O:570:TYR:HE2	1.82	0.45
2:P:391:TYR:HB3	2:P:462:ARG:HH11	1.72	0.45
1:B:114[B]:CYS:CB	1:B:208:ILE:HG21	2.47	0.45
1:B:573:LYS:HE2	1:B:671:CYS:O	2.17	0.45
2:M:23:ARG:NH1	11:M:1046:HOH:O	2.20	0.45
2:O:652:ILE:HA	2:O:657:PHE:CE2	2.52	0.45
2:N:613:ILE:O	2:N:671:PRO:HD3	2.17	0.44
2:P:391:TYR:HB3	2:P:462:ARG:HH12	1.76	0.44
1:B:114[B]:CYS:HB3	1:B:208:ILE:HG21	1.98	0.44
2:M:247:ARG:HA	2:M:247:ARG:HD2	1.52	0.44
2:O:419:HIS:HE1	2:O:421:GLY:O	2.01	0.44
2:O:515:ASN:O	2:O:575:SER:HB2	2.17	0.44
2:P:246:ARG:HG2	2:P:246:ARG:NH1	2.30	0.44
2:P:576:ASN:O	2:P:577:ARG:HB2	2.17	0.44
1:A:315:ILE:HG12	1:A:331:VAL:CG1	2.47	0.44
1:C:615:LEU:HD23	1:C:615:LEU:C	2.37	0.44
2:N:16:LYS:HE2	2:N:16:LYS:HB3	1.75	0.44
2:O:505:SER:HB3	2:O:570:TYR:CE2	2.52	0.44
1:C:587:LYS:HB3	5:C:900:CYN:C	2.48	0.44
1:D:68:CYS:HB2	1:D:97:ILE:CG2	2.46	0.44
2:O:344:GLY:O	2:O:346:ARG:HD3	2.18	0.44
1:A:331:VAL:HG13	1:A:332:THR:N	2.32	0.44
2:N:604:ILE:HG13	2:N:604:ILE:H	1.63	0.44
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.47	0.44
2:O:399:PHE:C	2:O:399:PHE:CD2	2.90	0.44
2:O:372:ASP:CG	2:O:440:ARG:HG3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:482:ARG:HA	2:O:485:TYR:HE2	1.69	0.44
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.53	0.44
2:P:113:ILE:O	2:P:117[A]:ARG:HG3	2.17	0.44
2:M:481:ALA:HB1	2:M:485:TYR:CZ	2.53	0.44
2:N:579:LEU:HD11	2:N:593:THR:HG21	1.99	0.44
2:P:453:LYS:HG3	2:P:463:VAL:CG2	2.47	0.44
2:P:459:ILE:HD13	2:P:542:ILE:HB	2.00	0.44
2:P:626:MET:HB2	2:P:631:LEU:HD22	1.99	0.44
1:C:213:SER:OG	1:D:209:HIS:HD2	2.00	0.44
1:D:293:GLN:NE2	1:D:296:ARG:HH11	2.16	0.44
2:M:408:HIS:CD2	2:M:419:HIS:ND1	2.78	0.44
2:N:683:VAL:HG13	2:N:693:GLU:HG3	2.00	0.44
2:O:169:LEU:HD13	2:O:193:LEU:HD21	2.00	0.44
6:D:963:GOL:H2	2:P:27:HIS:HE1	1.83	0.44
2:P:460:VAL:CG1	2:P:463:VAL:HG22	2.47	0.44
2:P:721:PRO:O	2:P:725:MET:HG3	2.18	0.44
2:P:595:CYS:HB2	9:P:953:ACT:H1	1.98	0.44
1:D:114:CYS:CA	11:D:1014:HOH:O	2.66	0.44
1:D:284:ASN:HD21	1:D:286:LEU:HG	1.83	0.44
2:M:320:LEU:HB3	2:M:321:PRO:HD2	2.00	0.44
2:N:246:ARG:C	2:N:247:ARG:HD2	2.38	0.43
2:N:350:PHE:CD1	2:N:350:PHE:C	2.92	0.43
2:O:340:VAL:HG22	2:O:373:ILE:HD12	2.00	0.43
2:O:425:ILE:HD12	2:O:426:ASN:HA	1.98	0.43
2:O:484:LYS:HD3	2:O:484:LYS:HA	1.64	0.43
2:O:715:LEU:HD22	2:O:720:HIS:CD2	2.53	0.43
2:P:340:VAL:HG21	2:P:376:ILE:HD11	2.00	0.43
2:P:553:LYS:HG2	2:P:564:TRP:NE1	2.33	0.43
2:O:425:ILE:CA	2:O:426:ASN:ND2	2.80	0.43
2:O:657:PHE:CZ	2:O:658:ILE:CD1	3.01	0.43
2:P:339:TYR:CE1	2:P:378:GLU:HG3	2.52	0.43
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.00	0.43
2:M:366:ILE:HA	2:M:465:VAL:O	2.19	0.43
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.54	0.43
2:O:658:ILE:HG22	2:O:661:ASP:HB2	2.00	0.43
2:P:489:ASP:O	2:P:493:ARG:HB2	2.17	0.43
2:M:670:MET:HE3	2:M:674:LEU:HB3	1.99	0.43
2:O:347:THR:OG1	2:O:382:LEU:O	2.33	0.43
2:O:725:MET:O	2:O:726:ASP:C	2.56	0.43
2:O:395:MET:HB3	2:O:396:GLN:H	1.56	0.43
2:O:423:ARG:CB	2:O:424:ASN:HD22	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:557:ILE:HD11	2:O:565:LYS:HB2	1.99	0.43
2:O:626:MET:HB2	2:O:631:LEU:HD13	1.99	0.43
1:C:114:CYS:CA	11:C:1383:HOH:O	2.66	0.43
2:O:658:ILE:O	2:O:658:ILE:CG2	2.65	0.43
2:P:423:ARG:HH21	2:P:488:ARG:HH12	1.66	0.43
1:B:200:THR:OG1	1:B:201:HIS:HD2	2.00	0.43
6:D:963:GOL:H2	2:P:27:HIS:CE1	2.54	0.43
2:P:565:LYS:HD3	2:P:565:LYS:O	2.19	0.43
1:A:118:ASN:OD1	1:A:209:HIS:HE1	2.01	0.43
1:B:284:ASN:HD22	1:B:284:ASN:C	2.21	0.43
1:C:284:ASN:HD22	1:C:285:PRO:N	2.17	0.43
1:D:114:CYS:SG	1:D:209:HIS:CD2	3.12	0.43
2:P:400:GLU:OE2	2:P:484:LYS:HE2	2.13	0.43
2:O:383:PRO:HB2	2:O:474:VAL:HG21	2.01	0.43
1:A:278:PHE:HB3	1:A:312:LEU:HD23	2.00	0.43
1:A:550:CYS:CB	5:A:900:CYN:N	2.82	0.43
1:C:176:ARG:O	1:C:207:GLY:HA3	2.19	0.43
2:M:164:LYS:HD3	2:M:298:TYR:CE1	2.54	0.43
2:P:272:THR:HG22	2:P:272:THR:O	2.19	0.43
2:P:342:MET:CG	2:P:384:LEU:HD22	2.40	0.43
2:P:400:GLU:OE1	2:P:484:LYS:HE3	2.18	0.43
1:B:220:HIS:HD2	1:B:221:MET:O	2.01	0.42
2:M:640[A]:GLN:HA	11:M:906:HOH:O	2.19	0.42
2:O:353:VAL:HG22	2:O:388:VAL:HB	2.00	0.42
2:O:393:ARG:HG3	2:O:394:LYS:N	2.31	0.42
2:O:532:SER:H	2:O:535:ASP:HB2	1.84	0.42
2:O:589:GLU:C	2:O:591:PRO:HD3	2.38	0.42
2:O:669:TRP:HA	2:O:700:ALA:O	2.19	0.42
2:P:471:GLU:HA	2:P:474:VAL:HG12	2.01	0.42
1:B:515:ASN:HA	1:B:518:THR:HG23	2.01	0.42
1:C:442:THR:HG21	1:C:537:ILE:HD11	2.00	0.42
2:M:61:TYR:HD1	2:M:66:ARG:HD2	1.84	0.42
2:N:247:ARG:HD2	2:N:247:ARG:HA	1.82	0.42
2:O:572:TYR:HA	2:O:579:LEU:O	2.18	0.42
2:P:448:LEU:O	2:P:452:MET:HG2	2.18	0.42
2:P:541:GLU:H	2:P:541:GLU:HG2	1.63	0.42
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.33	0.42
1:C:615:LEU:O	1:C:615:LEU:HD23	2.19	0.42
1:D:2:PRO:N	1:D:625:SER:HG	2.17	0.42
2:P:486:LYS:H	2:P:486:LYS:HG2	1.71	0.42
1:B:122:HIS:HD2	11:B:925:HOH:O	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ILE:HG13	1:B:195:LYS:HG3	2.01	0.42
1:B:299:GLU:O	1:B:303:LYS:HG3	2.19	0.42
2:M:702:GLU:H	2:M:702:GLU:HG3	1.31	0.42
2:N:384:LEU:HA	2:N:468:PHE:O	2.19	0.42
2:M:272:THR:O	2:M:272:THR:HG22	2.19	0.42
2:N:64:VAL:HG23	2:N:220:ASN:HB3	2.01	0.42
2:O:3:ASP:O	2:O:6:LYS:HG2	2.20	0.42
2:P:287:GLN:NE2	2:P:289:PRO:HD3	2.34	0.42
1:B:238:ALA:O	1:B:241:ASP:HB3	2.20	0.42
1:D:208:ILE:HG21	11:D:1014:HOH:O	2.19	0.42
2:M:339:TYR:HD2	2:M:340:VAL:CG2	2.32	0.42
2:P:7:ILE:HD13	2:P:245:ARG:HG3	2.02	0.42
1:B:217:ASN:O	1:B:223:MET:HG3	2.19	0.42
1:C:98:VAL:HG13	1:C:610:VAL:HA	2.02	0.42
2:N:247:ARG:HD2	2:N:247:ARG:N	2.32	0.42
2:O:439:PHE:O	2:O:440:ARG:HD3	2.20	0.42
1:A:394:ILE:HG23	1:A:395:GLU:N	2.35	0.42
1:D:128:ALA:HA	1:D:160:LEU:HD22	2.02	0.42
1:D:28:THR:OG1	1:D:477:GLN:NE2	2.53	0.42
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.54	0.42
1:B:571:THR:N	1:B:572:PRO:CD	2.83	0.42
2:N:353:VAL:HG22	2:N:388:VAL:HB	2.01	0.42
2:O:352:LEU:CD1	2:O:481:ALA:HA	2.47	0.42
1:D:339:LEU:HD13	1:D:339:LEU:HA	1.87	0.41
2:M:426:ASN:C	2:M:426:ASN:HD22	2.23	0.41
2:O:7:ILE:HD13	2:O:245:ARG:HD2	2.00	0.41
2:O:411:ILE:HG21	2:O:428:LEU:CD1	2.50	0.41
1:D:414:SER:O	1:D:415:ASN:O	2.39	0.41
2:M:384:LEU:HD11	2:M:467:ILE:HG23	2.01	0.41
2:O:266:ALA:HB1	2:O:276:VAL:HG21	2.01	0.41
2:O:307:GLU:HG3	2:O:308:THR:N	2.34	0.41
2:P:423:ARG:HH21	2:P:488:ARG:HH11	1.62	0.41
2:P:583:CYS:SG	2:P:589:GLU:HG2	2.60	0.41
2:N:262:LYS:HG3	11:N:2270:HOH:O	2.20	0.41
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.55	0.41
2:O:347:THR:HA	2:O:348:PRO:HD2	1.82	0.41
2:O:395:MET:O	2:O:396:GLN:CB	2.67	0.41
2:O:431:SER:OG	2:O:434:ALA:HB2	2.20	0.41
2:O:613:ILE:O	2:O:671:PRO:HD3	2.20	0.41
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.84	0.41
1:A:529:LYS:HE2	11:A:1060:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASN:ND2	1:B:286:LEU:H	2.18	0.41
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.56	0.41
2:O:534:LEU:N	2:O:534:LEU:HD12	2.36	0.41
2:P:382:LEU:HG	2:P:469:THR:HB	2.02	0.41
1:B:374:THR:HA	1:B:386:ILE:O	2.21	0.41
1:B:394:ILE:HG23	1:B:395:GLU:H	1.85	0.41
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.51	0.41
1:D:510:LEU:O	1:D:543:PRO:HD2	2.20	0.41
2:M:568:ASN:ND2	2:M:581:GLN:HE21	2.19	0.41
2:O:505:SER:CB	2:O:570:TYR:HE2	2.33	0.41
2:P:169:LEU:HG	2:P:193:LEU:HD21	2.02	0.41
2:P:390:ILE:HD13	2:P:463:VAL:HG13	2.02	0.41
2:P:602:MET:HE2	2:P:647:ILE:CG2	2.51	0.41
1:B:447:ASN:ND2	1:B:566:ASP:OD2	2.54	0.41
1:D:496:VAL:HA	1:D:545:PHE:O	2.21	0.41
2:M:86:LYS:HD3	2:M:86:LYS:HA	1.83	0.41
2:O:684:ARG:HH11	2:O:685:ARG:HG2	1.85	0.41
1:B:483:THR:HB	1:B:638:PRO:HB2	2.02	0.41
1:D:28:THR:HG21	1:D:33:VAL:HG12	2.02	0.41
2:M:122:LYS:HD2	2:M:125:GLU:OE1	2.20	0.41
2:M:383:PRO:HG2	2:M:469:THR:O	2.20	0.41
2:P:383:PRO:O	2:P:469:THR:HA	2.21	0.41
2:P:496:THR:OG1	2:P:499:THR:HG23	2.20	0.41
1:A:370:ARG:NH1	1:A:370:ARG:HG2	2.31	0.41
1:A:370:ARG:HH11	1:A:370:ARG:CG	2.33	0.41
1:A:603:HIS:HA	1:A:633:ILE:O	2.21	0.41
2:M:229:PHE:CD1	9:M:953:ACT:H2	2.56	0.41
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.85	0.41
2:P:281:PRO:HB3	2:P:296:GLU:OE1	2.20	0.41
2:O:478:MET:CE	2:O:478:MET:O	2.67	0.41
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.51	0.40
2:N:204:TYR:CE1	2:N:331:GLU:HB2	2.56	0.40
2:O:199:LYS:HZ2	2:O:199:LYS:HG3	1.51	0.40
2:P:219:ALA:O	2:P:223:LEU:HG	2.21	0.40
2:P:701:ASP:N	2:P:704:ILE:HD13	2.36	0.40
1:B:370:ARG:NE	11:B:2057:HOH:O	2.30	0.40
1:D:235:ILE:HG23	1:D:597:SER:OG	2.21	0.40
2:N:372:ASP:OD1	2:N:373:ILE:N	2.47	0.40
2:N:560:ILE:N	2:N:560:ILE:CD1	2.85	0.40
1:C:216:VAL:HG12	1:D:108:THR:HA	2.02	0.40
1:C:298:MET:HB3	1:C:298:MET:HE3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:324:PHE:HA	2:M:413:TYR:O	2.22	0.40
2:N:10:GLY:N	11:N:1249:HOH:O	2.28	0.40
2:O:425:ILE:H	2:O:426:ASN:ND2	2.19	0.40
2:O:612:MET:HB3	2:O:669:TRP:HB3	2.03	0.40
2:P:358:GLU:O	2:P:359:SER:HB3	2.21	0.40
2:P:720:HIS:HA	2:P:721:PRO:HD2	1.93	0.40
1:A:105:MET:HE3	1:A:105:MET:HB3	1.91	0.40
1:A:482:LEU:HA	1:A:482:LEU:HD22	1.90	0.40
1:B:118:ASN:C	1:B:118:ASN:HD22	2.25	0.40
2:N:721:PRO:O	2:N:725:MET:HG3	2.21	0.40
2:O:144:PHE:CE1	2:O:205:ILE:HG12	2.56	0.40
2:P:342:MET:HB3	2:P:382:LEU:O	2.22	0.40
1:C:62:GLY:HA3	3:C:700:SF4:S4	2.61	0.40
2:M:657:PHE:O	2:M:658:ILE:C	2.60	0.40
2:O:340:VAL:HG21	2:O:441:PHE:CZ	2.48	0.40
2:P:66:ARG:O	2:P:70:GLY:HA2	2.22	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	676/673 (100%)	651 (96%)	23 (3%)	2 (0%)	41	37
1	B	678/673 (101%)	653 (96%)	23 (3%)	2 (0%)	41	37
1	C	674/673 (100%)	648 (96%)	25 (4%)	1 (0%)	51	53
1	D	671/673 (100%)	645 (96%)	22 (3%)	4 (1%)	25	18
2	M	730/728 (100%)	697 (96%)	28 (4%)	5 (1%)	22	15
2	N	727/728 (100%)	700 (96%)	22 (3%)	5 (1%)	22	15
2	O	727/728 (100%)	650 (89%)	51 (7%)	26 (4%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	728/728 (100%)	684 (94%)	37 (5%)	7 (1%)	15	9
All	All	5611/5604 (100%)	5328 (95%)	231 (4%)	52 (1%)	17	11

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	267	ASN
1	B	415	ASN
1	D	415	ASN
1	D	416	ARG
2	N	316	ILE
2	O	315	LYS
2	O	335	LYS
2	O	395	MET
2	O	426	ASN
2	O	427	TRP
2	O	727	PRO
2	O	728	ILE
2	P	359	SER
1	A	415	ASN
1	C	267	ASN
1	D	267	ASN
1	D	417	PRO
2	M	315	LYS
2	N	315	LYS
2	O	187	ASP
2	O	360	GLU
2	O	363	ASP
2	O	366	ILE
2	O	396	GLN
2	O	397	ALA
2	O	400	GLU
2	O	423	ARG
2	O	449	VAL
2	O	470	ASP
2	O	722	ALA
2	P	458	ALA
2	M	187	ASP
2	M	596	GLY
2	N	187	ASP
2	O	348	PRO

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Mol	Chain	Res	Type
2	O	361	ILE
2	O	436	ALA
2	P	187	ASP
2	M	228	MET
2	N	228	MET
2	N	596	GLY
2	O	316	ILE
2	O	364	GLY
2	O	553	LYS
2	P	596	GLY
2	P	345	ASN
2	M	658	ILE
2	P	489	ASP
2	O	658	ILE
2	O	726	ASP
2	P	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	547/542 (101%)	530 (97%)	17 (3%)	40	39
1	B	549/542 (101%)	534 (97%)	15 (3%)	44	46
1	C	543/542 (100%)	530 (98%)	13 (2%)	49	51
1	D	541/542 (100%)	529 (98%)	12 (2%)	52	55
2	M	614/610 (101%)	581 (95%)	33 (5%)	22	18
2	N	611/610 (100%)	571 (94%)	40 (6%)	17	12
2	O	611/610 (100%)	540 (88%)	71 (12%)	5	2
2	P	612/610 (100%)	557 (91%)	55 (9%)	9	5
All	All	4628/4608 (100%)	4372 (94%)	256 (6%)	21	17

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	118	ASN
1	A	148	ARG
1	A	159	VAL
1	A	206	PHE
1	A	284	ASN
1	A	395	GLU
1	A	411	ARG
1	A	416	ARG
1	A	418	VAL
1	A	426	ARG
1	A	470	CYS
1	A	482	LEU
1	A	518	THR
1	A	636	MET
1	A	647	ASP
1	A	656	LEU
1	B	27	ARG
1	B	77	ARG
1	B	118	ASN
1	B	153	GLU
1	B	206	PHE
1	B	284	ASN
1	B	411	ARG
1	B	413	GLU
1	B	415	ASN
1	B	416	ARG
1	B	482	LEU
1	B	518	THR
1	B	539	ILE
1	B	636	MET
1	B	656	LEU
1	C	27	ARG
1	C	81[A]	THR
1	C	81[B]	THR
1	C	118	ASN
1	C	206	PHE
1	C	284	ASN
1	C	359	SER
1	C	466	LEU
1	C	482	LEU
1	C	636	MET
1	C	647	ASP

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Mol	Chain	Res	Type
1	C	656	LEU
1	C	664	GLU
1	D	82	ASP
1	D	118	ASN
1	D	196	GLU
1	D	206	PHE
1	D	284	ASN
1	D	415	ASN
1	D	518	THR
1	D	530	ARG
1	D	539	ILE
1	D	636	MET
1	D	656	LEU
1	D	664	GLU
2	M	14	GLU
2	M	66	ARG
2	M	127	LEU
2	M	152	THR
2	M	164	LYS
2	M	169	LEU
2	M	238[A]	GLU
2	M	238[B]	GLU
2	M	245	ARG
2	M	247	ARG
2	M	254	TYR
2	M	262	LYS
2	M	318	LEU
2	M	342	MET
2	M	354	ARG
2	M	373	ILE
2	M	378	GLU
2	M	381	LYS
2	M	422	GLN
2	M	424	ASN
2	M	426	ASN
2	M	448	LEU
2	M	471	GLU
2	M	486	LYS
2	M	492	MET
2	M	571	LEU
2	M	604	ILE
2	M	672	LYS

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Mol	Chain	Res	Type
2	M	674	LEU
2	M	702	GLU
2	M	704	ILE
2	M	723	LEU
2	M	726	ASP
2	N	6	LYS
2	N	66	ARG
2	N	124	ASP
2	N	152	THR
2	N	174	LYS
2	N	245	ARG
2	N	247	ARG
2	N	254	TYR
2	N	262	LYS
2	N	284	GLU
2	N	312	LYS
2	N	315	LYS
2	N	316	ILE
2	N	318	LEU
2	N	319	ASP
2	N	331	GLU
2	N	332	SER
2	N	335	LYS
2	N	342	MET
2	N	354	ARG
2	N	373	ILE
2	N	424	ASN
2	N	425	ILE
2	N	426	ASN
2	N	440	ARG
2	N	448	LEU
2	N	475	LYS
2	N	492	MET
2	N	493	ARG
2	N	495	LEU
2	N	560	ILE
2	N	571	LEU
2	N	604	ILE
2	N	631	LEU
2	N	640	GLN
2	N	672	LYS
2	N	674	LEU

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Mol	Chain	Res	Type
2	N	702	GLU
2	N	704	ILE
2	N	729	MET
2	O	2	THR
2	O	3	ASP
2	O	6	LYS
2	O	14	GLU
2	O	66	ARG
2	O	71	GLU
2	O	96	PHE
2	O	125	GLU
2	O	127	LEU
2	O	166	SER
2	O	169	LEU
2	O	174	LYS
2	O	205	ILE
2	O	214	GLN
2	O	245	ARG
2	O	284	GLU
2	O	316	ILE
2	O	317	LYS
2	O	319	ASP
2	O	342	MET
2	O	345	ASN
2	O	346	ARG
2	O	347	THR
2	O	350	PHE
2	O	351	GLU
2	O	352	LEU
2	O	356	VAL
2	O	360	GLU
2	O	362	THR
2	O	367	GLU
2	O	376	ILE
2	O	378	GLU
2	O	380	SER
2	O	393	ARG
2	O	396	GLN
2	O	399	PHE
2	O	406	ARG
2	O	422	GLN
2	O	423	ARG

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Mol	Chain	Res	Type
2	O	424	ASN
2	O	425	ILE
2	O	426	ASN
2	O	427	TRP
2	O	440	ARG
2	O	442	LYS
2	O	460	VAL
2	O	473	LYS
2	O	478	MET
2	O	484	LYS
2	O	495	LEU
2	O	497	ASP
2	O	524	ARG
2	O	525	VAL
2	O	535	ASP
2	O	541	GLU
2	O	575	SER
2	O	579	LEU
2	O	584	LEU
2	O	586	THR
2	O	609	ASN
2	O	622	THR
2	O	631	LEU
2	O	672	LYS
2	O	687	VAL
2	O	689	GLU
2	O	693	GLU
2	O	718	LYS
2	O	723	LEU
2	O	724	THR
2	O	728	ILE
2	O	729	MET
2	P	66	ARG
2	P	96	PHE
2	P	124	ASP
2	P	152	THR
2	P	174	LYS
2	P	205	ILE
2	P	245	ARG
2	P	254	TYR
2	P	272	THR
2	P	284	GLU

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Mol	Chain	Res	Type
2	P	286	LYS
2	P	315	LYS
2	P	317	LYS
2	P	329	GLU
2	P	331	GLU
2	P	335	LYS
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	362	THR
2	P	365	LYS
2	P	373	ILE
2	P	405	ARG
2	P	419	HIS
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	442	LYS
2	P	448	LEU
2	P	462	ARG
2	P	466	THR
2	P	471	GLU
2	P	478	MET
2	P	480	VAL
2	P	483	GLU
2	P	486	LYS
2	P	491	ARG
2	P	492	MET
2	P	495	LEU
2	P	502	THR
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	549	GLN
2	P	554	GLU
2	P	565	LYS
2	P	598	PHE
2	P	605	LEU
2	P	631	LEU
2	P	650	THR
2	P	674	LEU
2	P	686	SER

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Mol	Chain	Res	Type
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 (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	164	GLN
1	A	201	HIS
1	A	209	HIS
1	A	217	ASN
1	A	220	HIS
1	A	284	ASN
1	A	477	GLN
1	A	515	ASN
1	A	622	GLN
1	A	639	GLN
1	B	201	HIS
1	B	209	HIS
1	B	217	ASN
1	B	220	HIS
1	B	260	GLN
1	B	284	ASN
1	B	447	ASN
1	B	477	GLN
1	C	9	HIS
1	C	122	HIS
1	C	201	HIS
1	C	209	HIS
1	C	220	HIS
1	C	260	GLN
1	C	284	ASN
1	C	368	HIS
1	C	477	GLN
1	C	622	GLN
1	D	201	HIS
1	D	209	HIS
1	D	220	HIS
1	D	260	GLN
1	D	284	ASN
1	D	293	GLN

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Mol	Chain	Res	Type
1	D	477	GLN
1	D	503	GLN
1	D	515	ASN
1	D	622	GLN
1	D	639	GLN
2	M	211	ASN
2	M	408	HIS
2	M	422	GLN
2	M	424	ASN
2	M	426	ASN
2	M	544	HIS
2	M	549	GLN
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	426	ASN
2	N	510	GLN
2	N	549	GLN
2	N	581	GLN
2	N	590	ASN
2	N	679	HIS
2	O	27	HIS
2	O	396	GLN
2	O	424	ASN
2	O	515	ASN
2	O	516	HIS
2	O	576	ASN
2	O	590	ASN
2	O	609	ASN
2	O	640	GLN
2	O	720	HIS
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	464	GLN

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Mol	Chain	Res	Type
2	P	590	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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 38 ligands modelled in this entry, 12 are monoatomic - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SF4	M	900	2	0,12,12	0.00	-	-		
5	CYN	A	900	-	0,1,1	0.00	-	-		
5	CYN	C	900	-	0,1,1	0.00	-	-		
3	SF4	D	750	1	0,12,12	0.00	-	-		
9	ACT	P	953	-	1,2,3	1.31	0	1,1,3	0.28	0
6	GOL	A	963	-	5,5,5	0.67	0	5,5,5	1.75	2 (40%)
5	CYN	B	900	-	0,1,1	0.00	-	-		
4	XCC	A	800	1,11	0,11,11	0.00	-	-		
6	GOL	D	963	-	5,5,5	0.66	0	5,5,5	1.32	1 (20%)
3	SF4	N	900	2	0,12,12	0.00	-	-		
3	SF4	P	900	2	0,12,12	0.00	-	-		
3	SF4	C	700	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SF4	B	750	1	0,12,12	0.00	-	-		
6	GOL	C	963	-	5,5,5	0.53	0	5,5,5	0.93	0
9	ACT	O	953	-	1,2,3	1.27	0	1,1,3	0.33	0
3	SF4	O	900	2	0,12,12	0.00	-	-		
3	SF4	A	700	1	0,12,12	0.00	-	-		
4	XCC	C	800	1,11	0,11,11	0.00	-	-		
4	XCC	B	800	1,11	0,11,11	0.00	-	-		
6	GOL	B	963	-	5,5,5	0.80	0	5,5,5	1.67	1 (20%)
3	SF4	A	750	1	0,12,12	0.00	-	-		
3	SF4	C	750	1	0,12,12	0.00	-	-		
9	ACT	M	953	-	1,2,3	1.19	0	1,1,3	0.57	0
9	ACT	N	953	-	1,2,3	1.25	0	1,1,3	0.25	0
5	CYN	D	900	-	0,1,1	0.00	-	-		
4	XCC	D	800	1,11	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
3	SF4	M	900	2	-	-	0/6/5/5
4	XCC	A	800	1,11	-	-	0/3/3/3
4	XCC	D	800	1,11	-	-	0/3/3/3
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
6	GOL	D	963	-	-	4/4/4/4	-
6	GOL	B	963	-	-	1/4/4/4	-
3	SF4	N	900	2	-	-	0/6/5/5
3	SF4	D	750	1	-	-	0/6/5/5
4	XCC	B	800	1,11	-	-	0/3/3/3
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
6	GOL	C	963	-	-	4/4/4/4	-
3	SF4	P	900	2	-	-	0/6/5/5
6	GOL	A	963	-	-	2/4/4/4	-
3	SF4	A	700	1	-	-	0/6/5/5
4	XCC	C	800	1,11	-	-	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	963	GOL	O2-C2-C3	-2.41	98.50	109.12
6	D	963	GOL	O1-C1-C2	-2.31	99.10	110.20
6	A	963	GOL	O1-C1-C2	-2.29	99.24	110.20
6	A	963	GOL	O2-C2-C3	-2.13	99.73	109.12

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	963	GOL	C1-C2-C3-O3
6	B	963	GOL	C1-C2-C3-O3
6	A	963	GOL	O1-C1-C2-C3
6	C	963	GOL	O1-C1-C2-C3
6	D	963	GOL	O1-C1-C2-C3
6	D	963	GOL	O2-C2-C3-O3
6	C	963	GOL	O1-C1-C2-O2
6	D	963	GOL	O1-C1-C2-O2
6	C	963	GOL	O2-C2-C3-O3
6	C	963	GOL	C1-C2-C3-O3
6	A	963	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	CYN	2	0
5	C	900	CYN	3	0
9	P	953	ACT	1	0
6	A	963	GOL	1	0
6	D	963	GOL	6	0
3	C	700	SF4	1	0
6	C	963	GOL	4	0
9	O	953	ACT	1	0
9	M	953	ACT	1	0
9	N	953	ACT	3	0
5	D	900	CYN	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	673/673 (100%)	-0.06	25 (3%) 41 49	14, 24, 42, 62	0
1	B	673/673 (100%)	-0.10	20 (2%) 50 59	14, 22, 39, 66	0
1	C	673/673 (100%)	-0.26	11 (1%) 72 77	18, 26, 41, 57	0
1	D	673/673 (100%)	-0.09	14 (2%) 63 71	19, 28, 43, 62	0
2	M	728/728 (100%)	-0.10	18 (2%) 57 65	16, 31, 58, 76	0
2	N	728/728 (100%)	-0.04	20 (2%) 54 63	16, 30, 57, 71	0
2	O	728/728 (100%)	1.97	318 (43%) 0 0	25, 62, 88, 123	0
2	P	728/728 (100%)	0.76	146 (20%) 1 1	19, 45, 79, 107	0
All	All	5604/5604 (100%)	0.28	572 (10%) 6 10	14, 29, 74, 123	0

All (572) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	481	ALA	13.3
2	O	380	SER	9.8
2	O	486	LYS	9.8
2	O	485	TYR	9.6
2	O	490	ASP	9.4
2	O	494	GLY	9.3
2	O	474	VAL	9.2
2	O	461	ASP	9.1
2	O	493	ARG	9.1
2	O	361	ILE	8.9
2	O	381	LYS	8.4
2	O	728	ILE	8.1
2	O	476	GLU	7.9
2	P	461	ASP	7.9
2	O	357	SER	7.8
2	O	712	LEU	7.8

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Mol	Chain	Res	Type	RSRZ
2	O	340	VAL	7.8
2	O	339	TYR	7.7
2	P	483	GLU	7.7
2	O	567	VAL	7.6
2	O	391	TYR	7.5
2	P	391	TYR	7.5
2	O	724	THR	7.5
2	O	658	ILE	7.4
2	P	485	TYR	7.3
2	O	729	MET	7.3
2	O	399	PHE	7.2
2	O	564	TRP	7.2
2	O	450	ALA	7.2
2	O	458	ALA	7.1
2	O	470	ASP	7.0
2	O	390	ILE	7.0
2	O	492	MET	6.9
2	O	725	MET	6.9
2	O	696	ILE	6.9
2	O	369	ILE	6.8
2	O	359	SER	6.8
2	O	384	LEU	6.8
2	O	542	ILE	6.6
2	O	333	ILE	6.6
2	O	653	VAL	6.6
2	O	379	GLY	6.6
2	O	468	PHE	6.5
2	P	728	ILE	6.5
2	O	407	ILE	6.4
2	O	342	MET	6.4
2	O	424	ASN	6.4
2	O	397	ALA	6.4
2	O	478	MET	6.4
2	O	560	ILE	6.4
2	O	574	ALA	6.3
2	O	479	GLU	6.3
2	P	487	GLU	6.2
2	O	316	ILE	6.2
2	O	356	VAL	6.2
2	O	472	ALA	6.2
2	O	376	ILE	6.1
2	O	348	PRO	6.1

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Mol	Chain	Res	Type	RSRZ
2	O	427	TRP	6.1
2	P	491	ARG	6.1
2	O	373	ILE	6.0
2	O	456	PHE	6.0
2	O	691	LEU	6.0
2	O	704	ILE	6.0
2	O	559	PRO	6.0
1	D	417	PRO	6.0
2	P	481	ALA	5.9
2	O	718	LYS	5.9
2	P	361	ILE	5.9
2	O	449	VAL	5.9
2	O	683	VAL	5.9
2	P	393	ARG	5.9
2	O	354	ARG	5.8
2	O	699	ILE	5.8
2	O	570	TYR	5.8
2	O	664	ILE	5.8
2	P	356	VAL	5.7
2	O	439	PHE	5.6
2	O	418	TRP	5.5
2	P	729	MET	5.5
2	O	695	PHE	5.5
2	P	552	PRO	5.5
2	O	566	SER	5.5
2	O	463	VAL	5.4
2	O	488	ARG	5.4
2	O	368	VAL	5.4
2	O	714	TYR	5.4
2	O	392	GLY	5.4
2	O	483	GLU	5.4
2	O	665	ALA	5.4
2	O	462	ARG	5.4
2	O	398	ASP	5.4
2	O	422	GLN	5.4
2	O	362	THR	5.4
2	P	355	THR	5.3
2	P	359	SER	5.3
2	P	348	PRO	5.3
2	O	363	ASP	5.3
2	O	657	PHE	5.3
2	O	690	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	416	ARG	5.2
2	O	722	ALA	5.2
2	P	493	ARG	5.2
2	P	369	ILE	5.2
2	O	347	THR	5.2
2	O	540	TYR	5.1
2	O	469	THR	5.1
2	P	492	MET	5.1
2	O	460	VAL	5.1
2	O	353	VAL	5.1
2	O	350	PHE	5.1
2	O	14	GLU	5.0
2	O	364	GLY	5.0
2	O	579	LEU	5.0
2	O	435	VAL	5.0
2	O	389	ASP	5.0
2	P	364	GLY	4.9
2	O	504	TYR	4.9
2	O	685	ARG	4.9
2	O	495	LEU	4.9
2	O	489	ASP	4.9
2	O	484	LYS	4.9
2	P	490	ASP	4.8
2	O	365	LYS	4.8
2	O	491	ARG	4.8
2	O	697	ASP	4.7
2	O	436	ALA	4.7
2	O	623	PRO	4.7
2	O	717	GLU	4.7
2	O	584	LEU	4.7
2	O	343	GLY	4.7
2	N	729	MET	4.7
2	O	668	VAL	4.7
2	O	727	PRO	4.7
2	O	533	TRP	4.7
2	P	458	ALA	4.7
2	O	314	THR	4.6
2	O	366	ILE	4.6
2	P	472	ALA	4.6
2	O	541	GLU	4.6
2	O	663	GLY	4.6
2	O	667	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
2	O	387	LEU	4.5
2	O	694	ASP	4.5
2	O	573	THR	4.5
1	A	107	LEU	4.5
2	O	465	VAL	4.5
2	O	423	ARG	4.5
2	O	723	LEU	4.5
2	O	6	LYS	4.5
2	O	692	GLY	4.5
2	P	358	GLU	4.5
2	O	475	LYS	4.5
2	P	572	TYR	4.5
2	O	425	ILE	4.5
2	P	542	ILE	4.5
2	O	426	ASN	4.4
2	O	375	GLN	4.4
2	O	440	ARG	4.4
2	P	474	VAL	4.4
2	O	377	PRO	4.4
2	O	716	GLU	4.4
2	O	451	LYS	4.4
2	O	684	ARG	4.4
2	P	704	ILE	4.3
2	P	392	GLY	4.3
2	O	715	LEU	4.3
2	O	713	PRO	4.3
2	P	712	LEU	4.3
2	O	655	LYS	4.3
2	P	354	ARG	4.3
2	O	666	ARG	4.3
2	O	693	GLU	4.3
2	P	314	THR	4.3
2	P	682	PHE	4.2
2	P	363	ASP	4.2
2	O	703	THR	4.2
2	O	679	HIS	4.2
2	P	362	THR	4.2
2	O	719	GLY	4.2
2	O	545	ALA	4.2
2	P	696	ILE	4.2
2	O	612	MET	4.2
2	O	583	CYS	4.1

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Mol	Chain	Res	Type	RSRZ
2	P	623	PRO	4.1
2	O	611	ILE	4.1
2	O	355	THR	4.1
2	P	368	VAL	4.1
2	P	390	ILE	4.1
2	O	608	CYS	4.1
2	O	401	GLY	4.1
2	P	694	ASP	4.1
1	A	104[A]	LEU	4.1
2	O	586	THR	4.1
1	A	106	ILE	4.1
2	O	400	GLU	4.0
2	O	651	TYR	4.0
2	P	425	ILE	4.0
2	O	319	ASP	4.0
2	O	543	ASN	4.0
2	O	334	ARG	4.0
2	O	698	LYS	4.0
2	M	729	MET	4.0
2	O	457	PRO	4.0
2	O	467	ILE	4.0
2	P	462	ARG	4.0
2	O	534	LEU	3.9
1	D	415	ASN	3.9
2	O	674	LEU	3.9
2	O	471	GLU	3.9
2	P	14	GLU	3.9
2	P	476	GLU	3.9
2	M	318	LEU	3.9
2	O	395	MET	3.9
2	M	314	THR	3.9
2	O	678	LEU	3.9
2	O	344	GLY	3.8
2	P	402	VAL	3.8
2	O	519	ILE	3.8
2	O	393	ARG	3.8
2	M	316	ILE	3.8
2	P	690	GLY	3.8
2	P	692	GLY	3.7
2	O	726	ASP	3.7
2	P	334	ARG	3.7
2	O	522	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
2	O	502	THR	3.7
2	O	336	GLY	3.7
2	O	428	LEU	3.7
1	B	107	LEU	3.7
2	O	605	LEU	3.7
2	O	613	ILE	3.7
1	A	415	ASN	3.7
2	O	670	MET	3.7
2	O	606	PRO	3.7
2	P	427	TRP	3.7
2	O	554	GLU	3.7
2	O	563	ILE	3.6
2	P	486	LYS	3.6
2	P	494	GLY	3.6
2	O	552	PRO	3.6
2	O	352	LEU	3.6
2	O	317	LYS	3.6
2	O	711	ILE	3.6
2	P	560	ILE	3.6
2	P	570	TYR	3.6
2	P	15	GLY	3.6
2	N	373	ILE	3.5
2	O	358	GLU	3.5
2	O	551	ILE	3.5
2	P	714	TYR	3.5
2	O	338	MET	3.5
2	O	477	TYR	3.5
2	O	466	THR	3.5
2	O	555	GLY	3.5
2	O	686	SER	3.5
2	P	460	VAL	3.5
2	P	470	ASP	3.5
2	O	635	ILE	3.5
1	C	104	LEU	3.5
2	O	360	GLU	3.4
2	O	442	LYS	3.4
2	O	645	MET	3.4
2	P	475	LYS	3.4
2	O	621	MET	3.4
2	O	682	PHE	3.4
2	O	498	GLU	3.4
1	B	539	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	O	631	LEU	3.4
2	O	374	ASP	3.4
2	O	577	ARG	3.4
2	O	383	PRO	3.4
2	O	721	PRO	3.4
2	O	520	VAL	3.4
2	O	580	GLU	3.4
2	O	394	LYS	3.3
2	O	15	GLY	3.3
2	O	480	VAL	3.3
2	O	482	ARG	3.3
2	O	367	GLU	3.3
2	O	587	LEU	3.3
2	P	387	LEU	3.3
2	O	669	TRP	3.3
2	O	708	VAL	3.3
2	O	453	LYS	3.3
2	P	423	ARG	3.3
2	O	572	TYR	3.3
2	P	367	GLU	3.3
2	O	349	ALA	3.3
2	O	585	TYR	3.3
2	O	707	THR	3.3
2	P	718	LYS	3.3
1	D	104	LEU	3.3
2	O	582	VAL	3.3
2	O	650	THR	3.2
2	P	477	TYR	3.2
2	P	684[A]	ARG	3.2
1	A	216	VAL	3.2
2	P	340	VAL	3.2
2	O	671	PRO	3.2
2	P	719	GLY	3.2
2	P	403	LEU	3.2
2	O	382	LEU	3.2
2	O	571	LEU	3.2
2	O	388	VAL	3.2
2	O	565	LYS	3.2
2	O	687	VAL	3.2
2	P	703	THR	3.2
2	O	581	GLN	3.1
2	O	487	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	O	550	PRO	3.1
2	O	9	GLU	3.1
2	P	353	VAL	3.1
2	P	724	THR	3.1
2	P	727	PRO	3.1
1	B	104[A]	LEU	3.1
1	C	230	LEU	3.1
1	B	537	ILE	3.1
2	P	468	PHE	3.1
1	B	538	GLU	3.1
2	O	385	GLY	3.1
2	P	544	HIS	3.1
2	O	609	ASN	3.1
1	C	106	ILE	3.1
2	O	3	ASP	3.1
2	O	709	ASP	3.1
1	B	536	ASN	3.0
2	N	468	PHE	3.0
2	P	350	PHE	3.0
2	P	565	LYS	3.0
2	O	659	SER	3.0
2	O	372	ASP	3.0
1	C	215	LEU	3.0
2	N	318	LEU	3.0
2	O	351	GLU	3.0
2	O	625	GLY	3.0
2	O	662	GLY	3.0
2	O	447	ILE	3.0
2	P	374	ASP	3.0
2	O	544	HIS	3.0
2	P	124	ASP	3.0
2	P	467	ILE	3.0
2	P	711	ILE	3.0
2	P	698	LYS	3.0
2	O	689	GLU	3.0
2	N	314	THR	3.0
2	P	488	ARG	3.0
2	O	517	VAL	3.0
2	P	399	PHE	3.0
2	O	720	HIS	3.0
2	N	346	ARG	2.9
2	O	464	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
2	P	715	LEU	2.9
1	A	108	THR	2.9
2	P	284	GLU	2.9
2	P	707	THR	2.9
1	B	106	ILE	2.9
2	M	14	GLU	2.9
2	O	341	GLU	2.9
2	P	695	PHE	2.9
1	D	215	LEU	2.9
2	N	348	PRO	2.9
2	O	652	ILE	2.9
2	P	660	ALA	2.9
1	B	216	VAL	2.8
1	C	216	VAL	2.8
2	O	124	ASP	2.8
1	B	219	ALA	2.8
2	O	700	ALA	2.8
2	P	566	SER	2.8
2	O	318	LEU	2.8
2	O	370	GLY	2.8
1	A	416	ARG	2.8
2	P	377	PRO	2.8
2	P	432	LYS	2.8
2	P	424	ASN	2.8
1	A	231	VAL	2.8
2	O	332	SER	2.8
2	O	335	LYS	2.8
2	O	656	LYS	2.8
2	P	16	LYS	2.8
2	O	459	ILE	2.8
2	O	378	GLU	2.8
2	P	484	LYS	2.8
2	P	567	VAL	2.7
2	O	2	THR	2.7
2	O	622	THR	2.7
2	O	681	GLU	2.7
1	A	230	LEU	2.7
2	P	721	PRO	2.7
2	P	722	ALA	2.7
2	P	687	VAL	2.7
2	N	316	ILE	2.7
2	O	396	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	215	LEU	2.7
2	P	335	LYS	2.7
2	O	345	ASN	2.7
2	O	496	THR	2.7
2	O	499	THR	2.7
1	D	368	HIS	2.7
2	O	614	THR	2.7
2	P	541	GLU	2.6
2	P	580	GLU	2.6
2	M	472	ALA	2.6
2	O	295	VAL	2.6
2	O	371	PRO	2.6
2	O	443	ASN	2.6
2	O	710	GLU	2.6
2	O	432	LYS	2.6
2	O	433	ASP	2.6
2	O	640	GLN	2.6
2	N	381	LYS	2.6
2	O	639	THR	2.6
2	O	672	LYS	2.6
1	A	215	LEU	2.6
2	N	470	ASP	2.6
2	P	357	SER	2.6
2	O	151	TRP	2.6
2	P	610	GLY	2.6
1	A	70	PHE	2.6
1	A	103	GLY	2.5
2	M	470	ASP	2.5
1	C	107	LEU	2.5
2	M	693	GLU	2.5
2	O	526	GLY	2.5
2	O	16	LYS	2.5
1	D	304	ALA	2.5
2	P	555	GLY	2.5
1	B	231	VAL	2.5
2	P	697	ASP	2.5
1	D	107	LEU	2.5
1	D	216	VAL	2.5
2	O	702	GLU	2.5
1	B	212	ILE	2.5
2	P	533	TRP	2.5
2	N	367	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	O	705	GLY	2.5
2	P	400	GLU	2.5
1	B	70	PHE	2.5
2	N	475	LYS	2.5
2	O	503	PHE	2.5
2	P	473	LYS	2.5
2	M	124	ASP	2.4
2	O	501	ASP	2.4
2	O	641	THR	2.4
2	O	313	LEU	2.4
2	O	402	VAL	2.4
2	O	454	GLU	2.4
2	O	680	ASP	2.4
2	P	13	PRO	2.4
2	P	395	MET	2.4
2	P	606	PRO	2.4
2	O	429	ARG	2.4
2	P	479	GLU	2.4
2	P	577	ARG	2.4
2	P	501	ASP	2.4
1	A	619	ILE	2.4
2	O	13	PRO	2.4
2	O	602	MET	2.4
1	C	109	GLY	2.4
2	O	610	GLY	2.4
2	P	503	PHE	2.4
1	A	228	VAL	2.4
1	C	231	VAL	2.4
2	N	474	VAL	2.4
2	O	576	ASN	2.4
2	P	554	GLU	2.4
2	P	693	GLU	2.4
1	A	590	ALA	2.4
2	N	472	ALA	2.4
2	P	573	THR	2.4
2	P	471	GLU	2.3
2	O	507	VAL	2.3
2	P	668	VAL	2.3
2	O	289	PRO	2.3
2	O	321	PRO	2.3
1	A	105	MET	2.3
2	P	333	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	589	ALA	2.3
2	O	592	MET	2.3
2	P	381	LYS	2.3
1	A	212	ILE	2.3
2	O	410	PHE	2.3
1	B	234	ALA	2.3
2	O	530	ALA	2.3
2	M	469	THR	2.3
1	B	591	ILE	2.3
2	P	661	ASP	2.3
2	N	391	TYR	2.3
2	P	553	LYS	2.3
2	O	548	ASN	2.3
2	O	634	MET	2.3
2	O	642	PRO	2.3
2	M	719	GLY	2.3
2	P	394	LYS	2.3
2	O	416	GLY	2.3
2	P	688	GLU	2.3
1	D	588	ALA	2.2
2	P	480	VAL	2.2
2	P	581	GLN	2.2
2	O	569	ASP	2.2
1	B	230	LEU	2.2
2	O	11	ALA	2.2
2	P	665	ALA	2.2
2	P	375	GLN	2.2
2	P	569	ASP	2.2
2	P	584	LEU	2.2
1	A	109	GLY	2.2
1	A	234	ALA	2.2
2	P	418	TRP	2.2
2	P	551	ILE	2.2
1	C	227	PRO	2.2
2	N	339	TYR	2.2
2	O	430	VAL	2.2
2	O	661	ASP	2.2
2	O	594	SER	2.2
2	M	713	PRO	2.2
2	P	384	LEU	2.2
2	O	549	GLN	2.2
1	A	102	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	O	677	PHE	2.2
2	M	345	ASN	2.2
1	B	112	ALA	2.2
2	P	389	ASP	2.2
2	P	469	THR	2.2
1	D	106	ILE	2.1
2	M	696	ILE	2.1
2	O	556	GLU	2.1
1	A	589	ALA	2.1
2	O	421	GLY	2.1
1	B	108	THR	2.1
1	A	591	ILE	2.1
2	O	647	ILE	2.1
2	P	376	ILE	2.1
2	O	508	LEU	2.1
2	M	317	LYS	2.1
1	C	102	VAL	2.1
2	P	701	ASP	2.1
1	B	590	ALA	2.1
1	D	413	GLU	2.1
2	O	660	ALA	2.1
2	P	365	LYS	2.1
2	O	557	ILE	2.1
2	O	403	LEU	2.1
2	O	405	ARG	2.1
2	M	16	LYS	2.1
2	N	11	ALA	2.1
2	P	622	THR	2.1
2	O	558	ASP	2.1
2	N	360	GLU	2.1
2	P	6	LYS	2.1
2	O	688	GLU	2.1
2	P	583	CYS	2.1
2	O	676	ASP	2.0
2	P	457	PRO	2.0
1	A	110	ALA	2.0
1	A	237	VAL	2.0
1	C	590	ALA	2.0
2	M	381	LYS	2.0
1	A	534	GLY	2.0
2	N	564	TRP	2.0
2	M	348	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	588	MET	2.0
2	N	145	GLY	2.0
2	O	246	ARG	2.0
2	P	482	ARG	2.0
2	O	654	SER	2.0
1	B	110	ALA	2.0
1	D	591	ILE	2.0
2	P	382	LEU	2.0
2	P	664	ILE	2.0
2	O	531	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
10	NA	O	730	1/1	0.69	0.07	64,64,64,64	0
9	ACT	O	953	3/4	0.86	0.41	109,109,109,109	0
9	ACT	P	953	3/4	0.86	0.52	75,75,76,76	0
10	NA	P	730	1/1	0.87	0.15	35,35,35,35	0
6	GOL	B	963	6/6	0.90	0.18	27,37,38,44	0
6	GOL	A	963	6/6	0.90	0.18	26,30,37,38	0
6	GOL	C	963	6/6	0.90	0.20	50,53,54,55	0
9	ACT	N	953	3/4	0.91	0.25	71,71,71,71	0
6	GOL	D	963	6/6	0.93	0.13	38,43,45,45	0
5	CYN	B	900	2/2	0.94	0.13	25,25,25,25	0
3	SF4	O	900	8/8	0.94	0.06	57,60,62,64	0
10	NA	N	730	1/1	0.95	0.09	26,26,26,26	0
9	ACT	M	953	3/4	0.95	0.23	55,55,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CYN	C	900	2/2	0.95	0.25	31,31,31,33	0
5	CYN	A	900	2/2	0.96	0.16	31,31,31,32	0
7	CU1	O	950	1/1	0.98	0.04	73,73,73,73	0
7	CU1	P	950	1/1	0.98	0.03	49,49,49,49	0
10	NA	M	1	1/1	0.98	0.08	28,28,28,28	0
8	NI	O	951	1/1	0.98	0.04	66,66,66,66	0
5	CYN	D	900	2/2	0.98	0.12	42,42,42,43	0
7	CU1	M	950	1/1	0.99	0.10	35,35,35,35	0
3	SF4	D	750	8/8	0.99	0.13	24,24,26,26	0
4	XCC	D	800	9/9	0.99	0.12	27,30,36,36	0
3	SF4	N	900	8/8	0.99	0.11	20,23,24,25	0
3	SF4	A	700	8/8	0.99	0.09	16,17,19,20	0
4	XCC	C	800	9/9	0.99	0.11	19,25,28,31	0
4	XCC	B	800	9/9	0.99	0.12	18,19,24,26	0
8	NI	P	951	1/1	0.99	0.04	41,41,41,41	0
3	SF4	C	750	8/8	0.99	0.10	26,27,28,29	0
3	SF4	P	900	8/8	0.99	0.05	38,41,42,42	0
3	SF4	C	700	8/8	0.99	0.09	24,29,31,31	0
3	SF4	M	900	8/8	0.99	0.11	20,22,23,23	0
4	XCC	A	800	9/9	0.99	0.12	21,22,25,26	0
7	CU1	N	950	1/1	0.99	0.09	34,34,34,34	0
8	NI	N	951	1/1	1.00	0.10	24,24,24,24	0
3	SF4	B	750	8/8	1.00	0.12	16,16,18,18	0
8	NI	M	951	1/1	1.00	0.09	24,24,24,24	0
3	SF4	A	750	8/8	1.00	0.13	17,17,18,19	0

## 6.5 Other polymers

There are no such residues in this entry.