Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 09:24 AM GMT

PDB ID	:	3I04
Title	:	Cyanide-bound structure of bifunctional carbon monoxide dehydrogenase/acetyl-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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

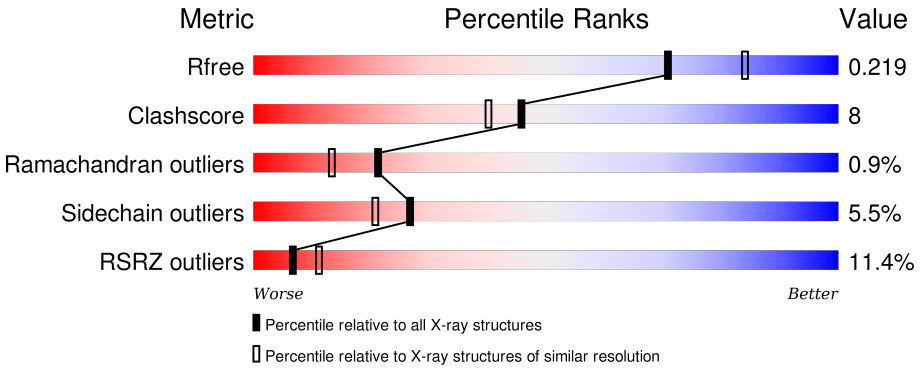
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 90% 9%
1	B	673	4% 89% 10%
1	C	673	2% 91% 8%
1	D	673	4% 88% 11%
2	M	728	3% 87% 11%

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Mol	Chain	Length	Quality of chain
2	N	728	3% 86% 11%
2	O	728	45% 68% 25% 6%
2	P	728	22% 78% 18%

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	X
6	GOL	B	963	-	-	-	X
6	GOL	C	963	-	-	X	-
6	GOL	D	963	-	-	X	-
9	ACT	M	953	-	-	-	X
9	ACT	N	953	-	-	X	X
9	ACT	O	953	-	-	-	X
9	ACT	P	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.

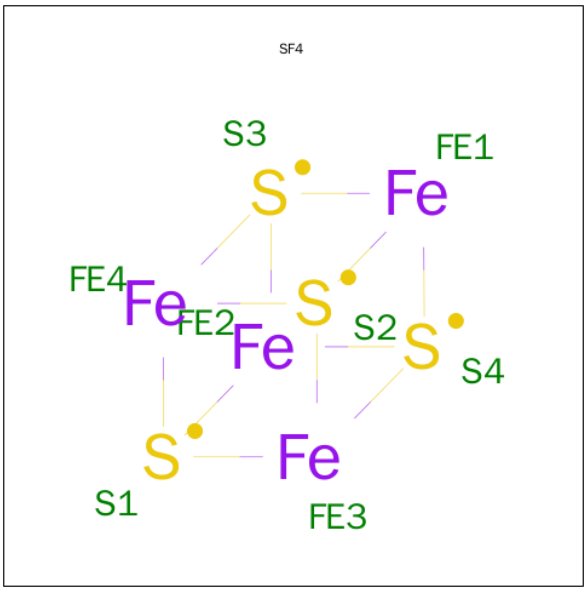
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

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.

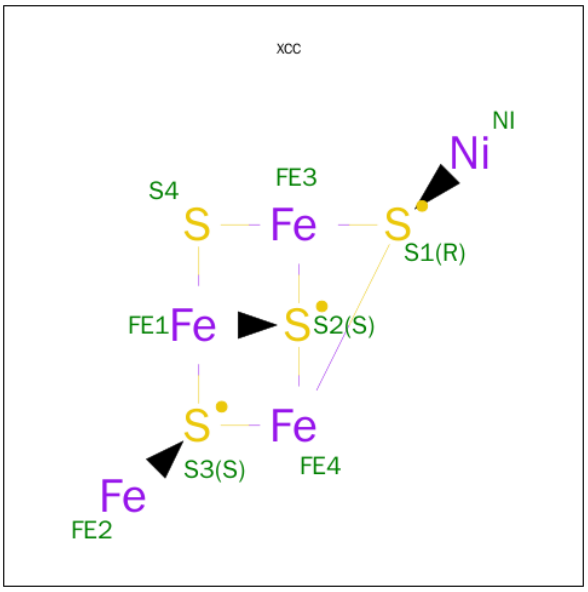
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5766	3695	962	1074	35			
2	N	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	O	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	P	728	Total	C	N	O	S	0	2	0
			5757	3690	963	1069	35			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



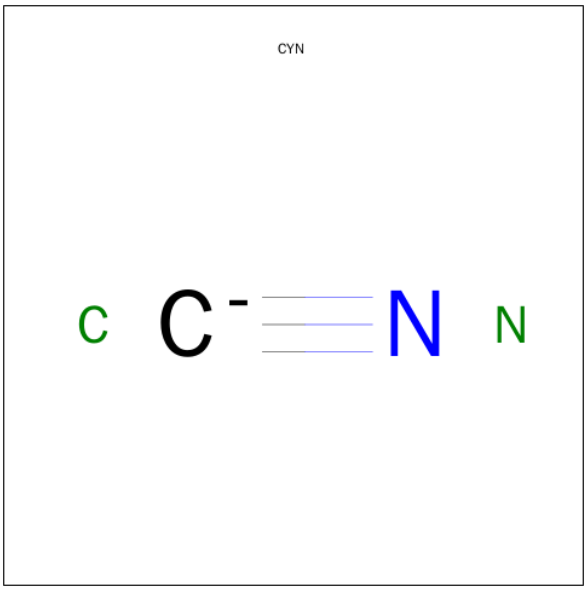
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 8 4 4	0	0
3	A	1	Total Fe S 8 4 4	0	0
3	B	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	C	1	Total Fe S 8 4 4	0	0
3	D	1	Total Fe S 8 4 4	0	0
3	M	1	Total Fe S 8 4 4	0	0
3	N	1	Total Fe S 8 4 4	0	0
3	O	1	Total Fe S 8 4 4	0	0
3	P	1	Total Fe S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

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe_4NiS_4).



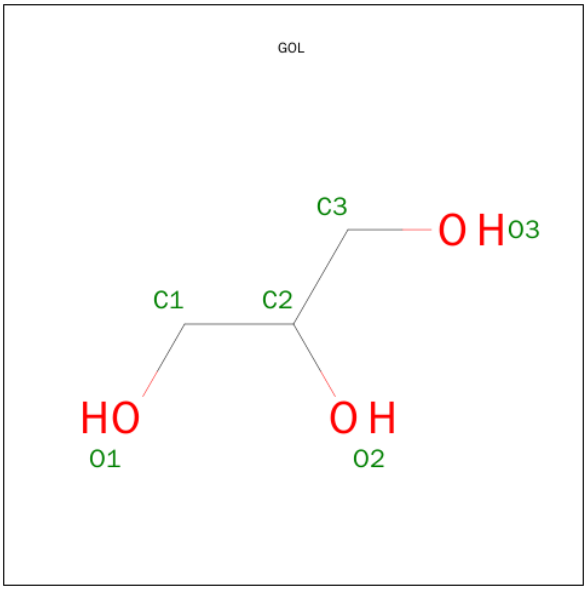
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- 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: $C_3H_8O_3$).



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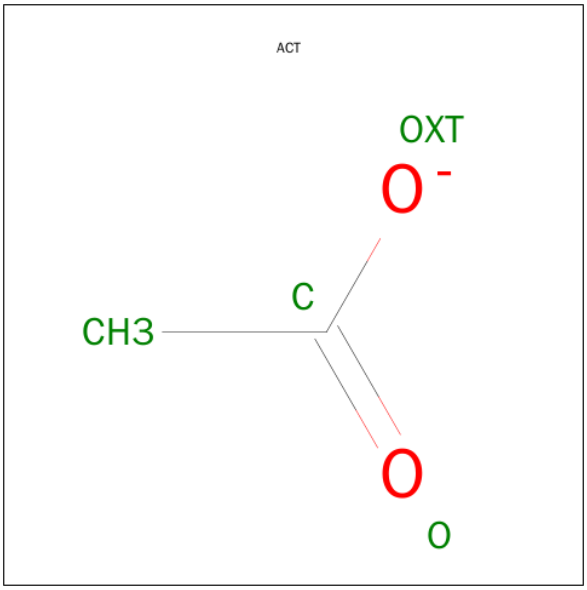
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	N	1	Total Cu 1 1	0	0
7	M	1	Total Cu 1 1	0	0

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

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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

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

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

- Molecule 11 is water.

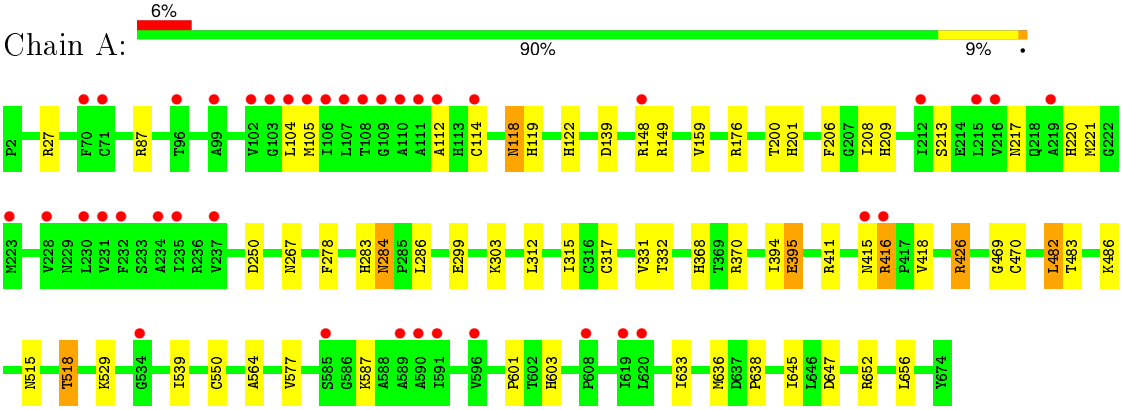
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	306	Total O 306 306	0	0
11	B	375	Total O 375 375	0	0
11	C	275	Total O 275 275	0	0
11	D	240	Total O 240 240	0	0
11	M	326	Total O 326 326	0	0
11	N	337	Total O 337 337	0	0
11	O	83	Total O 83 83	0	0
11	P	213	Total O 213 213	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

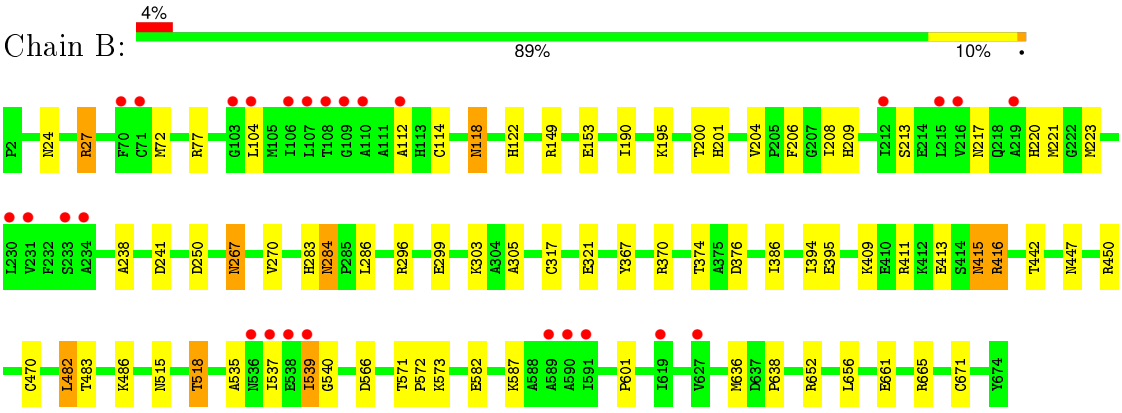
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

Chain A:



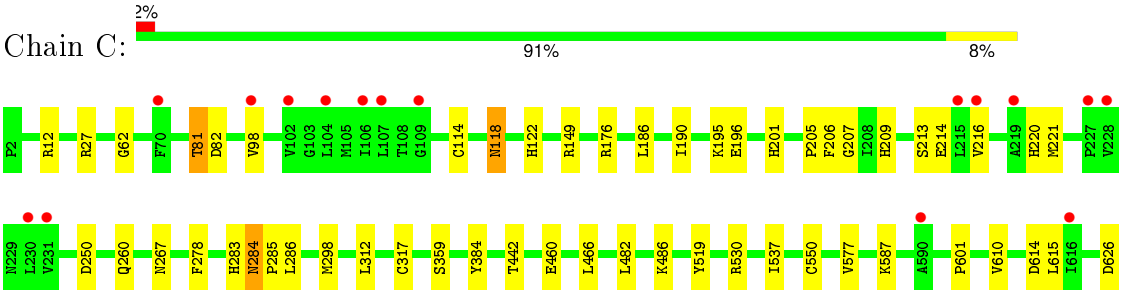
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

Chain B:

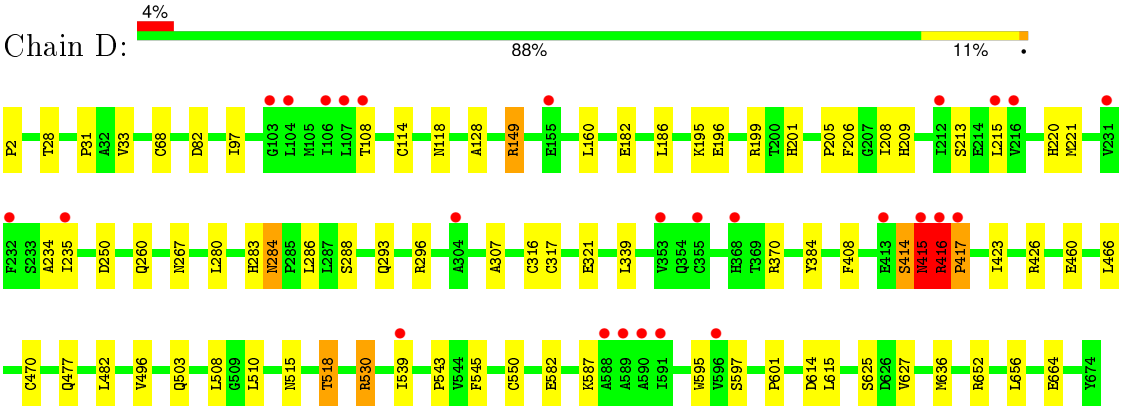


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

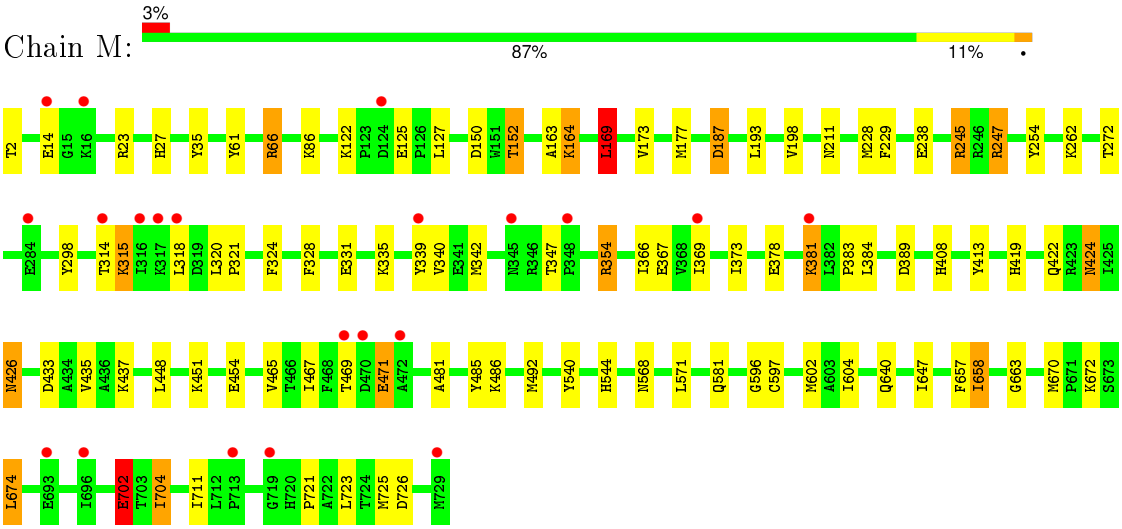
Chain C:



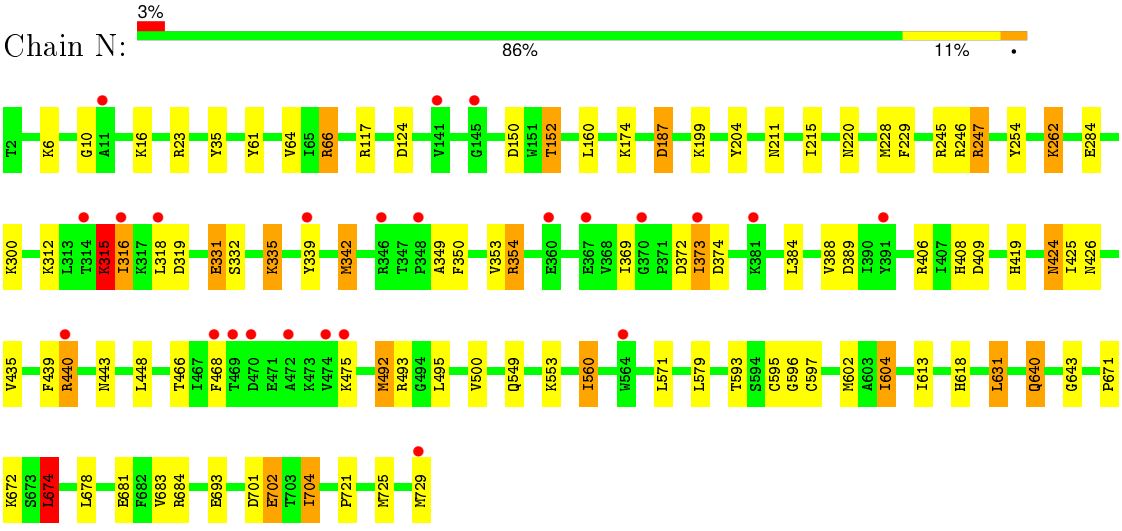
• Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



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

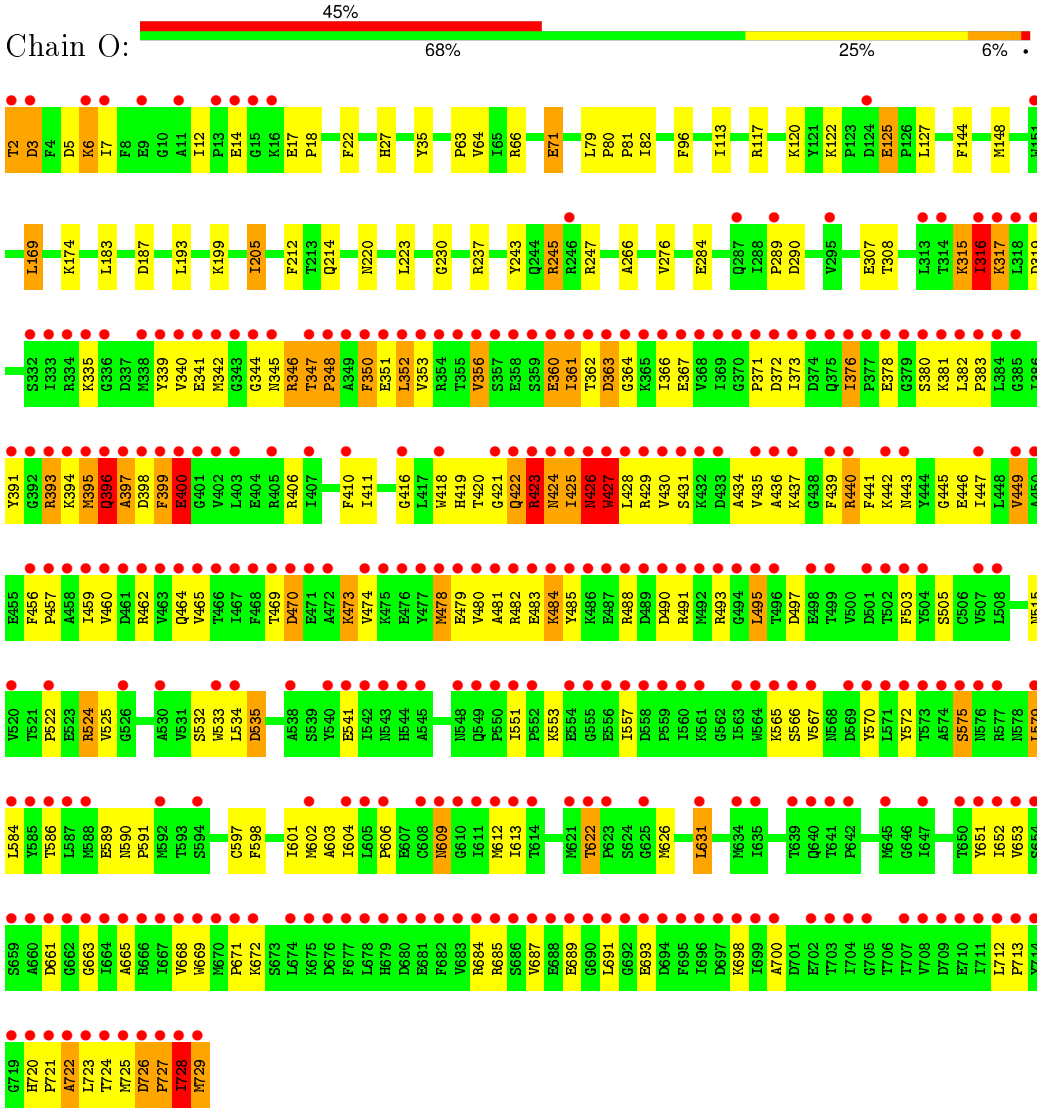


• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



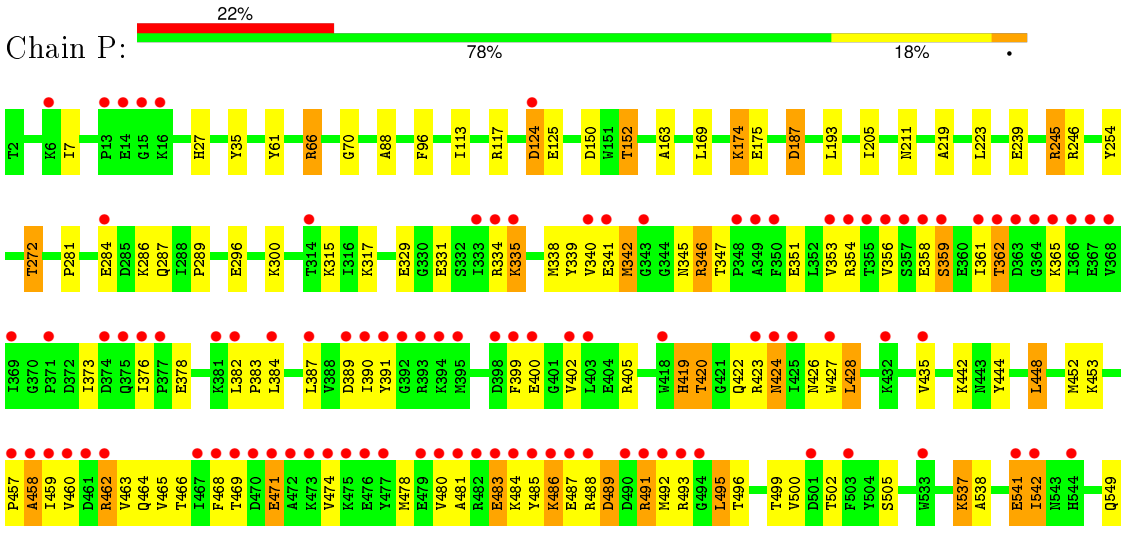
• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

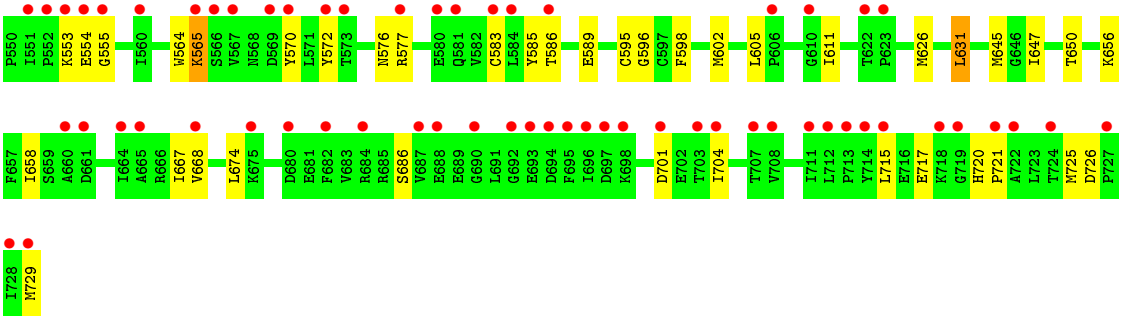
Chain O:



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

Chain P:




P550 I551 P552 K553 E554 G555 I560 W564 K565 S566 V567 N568 D569 Y570 L571 Y572 T573 N576 R577 E580 Q581 V582 C583 L584 Y585 T586 E589 C595 G596 C597 F598 M602 L605 P606 G610 I611 T622 P623 M626 L631 M645 G646 I647 T650 K656
F657 I658 S659 A660 D661 I664 A665 R666 I667 V668 L674 K675 D680 E681 F682 V683 R684 R685 S686 V687 E688 E689 G690 L691 G692 E693 D694 F695 I696 D697 K698 D701 E702 T703 I704 T707 V708 I711 L712 P713 Y714 L715 E716 E717 K718 G719 H720 P721 A722 L723 T724 M725 D726 P727
I728 M729

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 86.8 (48.40-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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 (5.23%)	DCC
Wilson B-factor (Å^2)	28.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 344234 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	45801	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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:424:ASN:O	2:O:425:ILE:CG2	2.30	0.77
2:O:376:ILE:HD12	2:O:382:LEU:HD21	1.63	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:O:376:ILE:CD1	2:O:382:LEU:HD21	2.17	0.74
2:M:335:LYS:HD2	2:M:335:LYS:H	1.52	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
2:P:602:MET:HE3	2:P:645:MET:CE	2.17	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: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:O:657:PHE:CE1	2:O:658:ILE:CD1	2.70	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:N:424:ASN:HD22	2:N:424:ASN:H	1.38	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:P:356:VAL:O	2:P:391:TYR:HB2	1.91	0.70
2:M:408:HIS:HD2	2:M:419:HIS:ND1	1.90	0.70
2:P:338:MET:HE1	2:P:341:GLU:CB	2.17	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: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
2:O:395:MET:CA	2:O:399:PHE:CZ	2.75	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: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
2:O:316:ILE:HG21	2:O:454:GLU:HG3	1.76	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
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:O:651:TYR:CD2	2:O:657:PHE:HD2	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:704:ILE:HD11	2:M:711:ILE:HA	1.76	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
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:485:TYR:HA	2:O:488:ARG:HE	1.58	0.67
2:O:653:VAL:O	2:O:685:ARG:HD2	1.94	0.67
2:N:150:ASP:OD2	2:N:152:THR:CG2	2.42	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
2:P:424:ASN:ND2	2:P:424:ASN:H	1.93	0.65
1:C:220:HIS:HE1	1:D:587:LYS:H	1.42	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
2:P:246:ARG:HG2	2:P:246:ARG:HH11	1.60	0.65
1:A:220:HIS:HD2	1:A:221:MET:O	1.80	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
2:O:424:ASN:N	2:O:424:ASN:HD22	1.96	0.64
2:O:420:THR:O	2:O:426:ASN:HA	1.98	0.64
1:A:220:HIS:HE1	1:B:587:LYS:H	1.46	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:P:341:GLU:CD	2:P:427:TRP:HE1	2.03	0.62
2:O:572:TYR:HD1	2:O:580:GLU:HB3	1.63	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:B:149:ARG:NH2	1:B:250:ASP:OD2	2.34	0.60
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.37	0.60
2:O:727:PRO:O	2:O:729:MET:N	2.35	0.60
1:C:220:HIS:HD2	1:C:221:MET:O	1.84	0.60
2:O:490:ASP:C	2:O:493:ARG:HG2	2.21	0.60
2:M:367:GLU:HG3	2:M:369:ILE:HD11	1.84	0.60
1:D:284:ASN:HD22	1:D:286:LEU:H	1.50	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
2:O:430:VAL:HG21	2:O:439:PHE:CE2	2.37	0.60
1:C:284:ASN:HD22	1:C:286:LEU:H	1.50	0.60
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.37	0.60
2:P:419:HIS:ND1	2:P:420:THR:N	2.49	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
2:N:354:ARG:CD	2:N:389:ASP:OD2	2.50	0.59
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.85	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
2:P:483:GLU:O	2:P:487:GLU:HB2	2.03	0.59
1:C:196[B]:GLU:OE2	2:O:120:LYS:NZ	2.36	0.59
2:N:229:PHE:HD1	9:N:953:ACT:H2	1.66	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:M:602:MET:HE2	2:M:657:PHE:CE2	2.34	0.58
1:B:442:THR:HG21	1:B:535:ALA:HA	1.83	0.58
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.33	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:O:425:ILE:C	2:O:426:ASN:CG	2.55	0.58
2:N:595:CYS:HB2	9:N:953:ACT:H1	1.84	0.58
2:O:346:ARG:NH1	2:O:427:TRP:CE2	2.65	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
2:O:18:PRO:HD2	2:O:22:PHE:CZ	2.38	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
2:O:324:PHE:CE2	2:O:451:LYS:HE2	2.39	0.57
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: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:D:614:ASP:H	6:D:963:GOL:H11	1.68	0.57
1:C:209:HIS:HD2	1:D:213:SER:OG	1.87	0.57
1:A:114[B]:CYS:SG	1:A:208:ILE:CG2	2.93	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
2:O:424:ASN:N	2:O:424:ASN:ND2	2.50	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: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
2:P:399:PHE:HE2	2:P:541:GLU:HG3	1.70	0.56
1:D:414:SER:O	1:D:415:ASN:C	2.40	0.56
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.40	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
2:O:424:ASN:C	2:O:425:ILE:HG23	2.25	0.56
2:O:356:VAL:HG23	2:O:361:ILE:CD1	2.36	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)
2:N:150:ASP:OD2	2:N:152:THR:HG22	2.06	0.55
1:B:447:ASN:HD22	1:B:450:ARG:HB2	1.72	0.55
2:P:602:MET:CE	2:P:647:ILE:HG21	2.36	0.55
2:N:335:LYS:H	2:N:335:LYS:CD	2.19	0.55
1:A:426:ARG:CZ	11:A:2027:HOH:O	2.54	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:O:418:TRP:O	2:O:428:LEU:HD13	2.06	0.55
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.07	0.55
2:M:163:ALA:HB2	2:M:169:LEU:HG	1.89	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:112:ALA:HA	1:B:217:ASN:HD22	1.72	0.54
1:A:368:HIS:NE2	1:A:416:ARG:HG3	2.23	0.54
2:O:480:VAL:O	2:O:484:LYS:HB2	2.07	0.54
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.36	0.54
1:A:122:HIS:HD2	11:A:926:HOH:O	1.90	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:O:479:GLU:O	2:O:483:GLU:HG3	2.07	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
1:A:119:HIS:CE1	11:A:1427:HOH:O	2.60	0.54
2:P:335:LYS:HD2	2:P:335:LYS:H	1.72	0.54
2:O:388:VAL:HG13	2:O:465:VAL:HG22	1.88	0.54
2:N:66:ARG:HD3	11:N:754:HOH:O	2.07	0.53
2:O:425:ILE:C	2:O:426:ASN:HD22	1.88	0.53
2:O:157:ALA:HB3	2:O:183:LEU:HD23	1.91	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
2:O:324:PHE:CZ	2:O:451:LYS:HE2	2.43	0.53
1:B:114[B]:CYS:SG	1:B:208:ILE:CG2	2.96	0.53
1:D:470:CYS:O	1:D:582:GLU:HB2	2.09	0.53
2:O:416:GLY:O	2:O:430:VAL:HA	2.09	0.53
2:P:457:PRO:O	2:P:458:ALA:HB2	2.08	0.53
1:D:260:GLN:NE2	11:D:1371:HOH:O	2.41	0.53
2:P:387:LEU:O	2:P:465:VAL:HA	2.09	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
2:N:618:HIS:CE1	2:N:702:GLU:HG2	2.43	0.52
2:N:349:ALA:HA	2:N:384:LEU:O	2.10	0.52
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.38	0.52
2:P:354:ARG:CD	2:P:356:VAL:HG13	2.31	0.52
2:N:681:GLU:HG2	2:N:684:ARG:HH21	1.75	0.52
2:P:602:MET:HE1	2:P:647:ILE:HG21	1.90	0.52
1:B:284:ASN:HD22	1:B:286:LEU:H	1.56	0.52
1:C:114:CYS:SG	1:C:209:HIS:NE2	2.83	0.52
2:O:503:PHE:O	2:O:551:ILE:N	2.28	0.52
2:N:199:LYS:HE3	2:N:204:TYR:OH	2.09	0.52
2:O:421:GLY:HA3	2:O:425:ILE:HD11	1.91	0.52
2:M:173:VAL:O	2:M:177:MET:HG3	2.10	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:O:80:PRO:HB2	2:O:81:PRO:HD3	1.92	0.51
2:M:314:THR:O	2:M:315:LYS:C	2.49	0.51
2:M:602:MET:CE	2:M:657:PHE:HE2	2.23	0.51
1:A:201:HIS:HE1	2:M:35:TYR:OH	1.94	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
2:P:602:MET:CE	2:P:645:MET:HE3	2.41	0.51
2:M:150:ASP:OD2	2:M:152:THR:CG2	2.57	0.51
1:C:81[B]:THR:HG23	1:C:82:ASP:OD2	2.09	0.51
2:O:668:VAL:HG12	2:O:720:HIS:CE1	2.46	0.51
2:O:478:MET:CE	2:O:478:MET:CA	2.72	0.51
1:A:213:SER:OG	1:B:209:HIS:HD2	1.94	0.51
2:P:61:TYR:HD1	2:P:66:ARG:HD2	1.76	0.51
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.91	0.51
2:M:339:TYR:HD2	2:M:340:VAL:HG22	1.75	0.51
2:P:419:HIS:C	2:P:419:HIS:ND1	2.64	0.51
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.46	0.51
2:O:590:ASN:N	2:O:591:PRO:HD3	2.25	0.51
2:O:658:ILE:HG23	2:O:661:ASP:HB2	1.93	0.51
1:B:470:CYS:O	1:B:582:GLU:HB2	2.11	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)
2:P:505:SER:HB3	2:P:570:TYR:CE2	2.46	0.50
1:D:317:CYS:O	1:D:321:GLU:HG2	2.11	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:P:339:TYR:CE1	2:P:435:VAL:HG11	2.47	0.50
2:N:640:GLN:HA	11:N:954:HOH:O	2.10	0.50
2:O:425:ILE:N	2:O:426:ASN:ND2	2.59	0.49
2:O:397:ALA:HA	2:O:400:GLU:OE1	2.12	0.49
2:P:124:ASP:OD1	2:P:125:GLU:OE1	2.29	0.49
2:O:657:PHE:O	2:O:663:GLY:HA2	2.12	0.49
1:A:515:ASN:ND2	1:A:518:THR:HG21	2.23	0.49
2:P:420:THR:O	2:P:420:THR:HG23	2.12	0.49
2:N:618:HIS:HE1	2:N:702:GLU:HG2	1.76	0.49
1:B:201:HIS:HE1	2:N:35:TYR:OH	1.95	0.49
2:O:456:PHE:N	2:O:457:PRO:HD3	2.27	0.49
1:D:370:ARG:HD2	1:D:384:TYR:CE2	2.47	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
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:B:394:ILE:HG23	1:B:395:GLU:N	2.28	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:C:577:VAL:HG11	1:C:645:ILE:HG23	1.95	0.49
1:B:305:ALA:HB1	1:B:409:LYS:HE3	1.95	0.49
2:O:346:ARG:HG3	2:O:381:LYS:HZ3	1.76	0.49
2:O:443:ASN:HA	2:O:446:GLU:OE2	2.12	0.49
2:O:411:ILE:HD13	2:O:428:LEU:HD11	1.93	0.49
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.28	0.49
2:P:481:ALA:HB1	2:P:485:TYR:CZ	2.48	0.49
2:P:351:GLU:OE2	2:P:426:ASN:ND2	2.46	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: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:N:61:TYR:HD1	2:N:66:ARG:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.96	0.48
2:N:374:ASP:HB3	2:N:440:ARG:HH21	1.77	0.48
2:O:425:ILE:O	2:O:425:ILE:HD12	2.02	0.48
2:M:568:ASN:HD21	2:M:581:GLN:HE21	1.61	0.48
2:O:396:GLN:NE2	2:O:398:ASP:HB2	2.25	0.48
1:D:615:LEU:H	6:D:963:GOL:C1	2.25	0.48
1:D:316:CYS:H	1:D:503:GLN:HE22	1.61	0.48
2:O:423:ARG:C	2:O:424:ASN:ND2	2.67	0.48
1:A:550:CYS:HB3	5:A:900:CYN:N	2.29	0.48
2:M:540:TYR:O	2:M:544:HIS:HD2	1.96	0.48
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.78	0.48
2:N:492:MET:HE2	11:N:1937:HOH:O	2.13	0.48
2:M:424:ASN:N	2:M:424:ASN:HD22	2.07	0.48
2:O:597:CYS:HB3	9:O:953:ACT:H1	1.96	0.48
2:N:315:LYS:HD2	2:N:315:LYS:H	1.77	0.48
1:A:201:HIS:CE1	2:M:35:TYR:OH	2.67	0.48
1:D:201:HIS:CE1	2:P:35:TYR:OH	2.67	0.48
2:O:289:PRO:O	2:O:290:ASP:HB2	2.12	0.48
1:A:104[A]:LEU:CD2	1:B:104[A]:LEU:HD22	2.43	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
2:O:372:ASP:O	2:O:376:ILE:HG12	2.13	0.48
2:N:602:MET:HB3	2:N:602:MET:HE2	1.75	0.48
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.95	0.48
2:O:350:PHE:CD1	2:O:481:ALA:HB2	2.49	0.47
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.44	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
1:D:284:ASN:HD22	1:D:284:ASN:C	2.18	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: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
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
1:A:482:LEU:CD1	1:A:486:LYS:HE3	2.45	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
2:M:657:PHE:O	2:M:663:GLY:HA2	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
1:B:267:ASN:O	1:B:270:VAL:HG22	2.15	0.46
2:O:113:ILE:O	2:O:117[A]:ARG:HG3	2.15	0.46
2:O:376:ILE:HD13	2:O:382:LEU:HD21	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: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:M:339:TYR:CG	2:M:435:VAL:HG21	2.49	0.46
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.51	0.46
1:A:482:LEU:HD13	1:A:486:LYS:HE3	1.97	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:O:439:PHE:CE1	2:O:443:ASN:HB2	2.51	0.46
2:N:604:ILE:HG13	2:N:643:GLY:O	2.16	0.46
1:B:661[A]:GLU:HG3	1:B:665:ARG:HH21	1.81	0.46
1:A:483:THR:HB	1:A:638:PRO:HB2	1.97	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: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
1:B:367:TYR:HA	1:B:416:ARG:HH12	1.81	0.46
2:O:566:SER:HB3	11:O:1472:HOH:O	2.16	0.46
1:D:201:HIS:HE1	2:P:35:TYR:OH	1.99	0.46
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.98	0.46
1:C:114:CYS:SG	1:C:209:HIS:CD2	3.09	0.45
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.50	0.45
2:N:674:LEU:HD22	2:N:678:LEU:HG	1.98	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
2:M:347:THR:CG2	2:M:381:LYS:HG3	2.47	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
2:O:339:TYR:HB3	2:O:373:ILE:HD11	1.99	0.45
1:B:201:HIS:CE1	2:N:35:TYR:OH	2.70	0.45
2:P:338:MET:HG2	2:P:339:TYR:H	1.81	0.45
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.99	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:C:614:ASP:H	6:C:963:GOL:H32	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:A:209:HIS:HD2	1:B:213:SER:CB	2.30	0.45
2:O:470:ASP:HB3	2:O:473:LYS:CB	2.47	0.45
2:N:342:MET:SD	2:N:342:MET:N	2.90	0.45
1:D:466:LEU:CD2	1:D:595:TRP:CZ2	2.97	0.45
2:P:391:TYR:HB3	2:P:462:ARG:HH11	1.72	0.45
2:O:505:SER:HB3	2:O:570:TYR:HE2	1.82	0.45
2:O:652:ILE:HA	2:O:657:PHE:CE2	2.52	0.45
1:B:114[B]:CYS:CB	1:B:208:ILE:HG21	2.47	0.45
2:M:23:ARG:NH1	11:M:1046:HOH:O	2.20	0.45
1:B:573:LYS:HE2	1:B:671:CYS:O	2.17	0.45
2:P:391:TYR:HB3	2:P:462:ARG:HH12	1.76	0.44
2:N:613:ILE:O	2:N:671:PRO:HD3	2.17	0.44
2:O:419:HIS:HE1	2:O:421:GLY:O	2.01	0.44
1:B:114[B]:CYS:HB3	1:B:208:ILE:HG21	1.98	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
2:M:247:ARG:HA	2:M:247:ARG:HD2	1.52	0.44
2:O:515:ASN:O	2:O:575:SER:HB2	2.17	0.44
2:O:505:SER:HB3	2:O:570:TYR:CE2	2.52	0.44
1:A:315:ILE:HG12	1:A:331:VAL:CG1	2.47	0.44
2:N:16:LYS:HE2	2:N:16:LYS:HB3	1.75	0.44
1:C:615:LEU:HD23	1:C:615:LEU:C	2.37	0.44
1:C:587:LYS:HB3	5:C:900:CYN:C	2.48	0.44
2:O:344:GLY:O	2:O:346:ARG:HD3	2.18	0.44
1:D:68:CYS:HB2	1:D:97:ILE:CG2	2.46	0.44
2:O:399:PHE:C	2:O:399:PHE:CD2	2.90	0.44
2:O:482:ARG:HA	2:O:485:TYR:HE2	1.69	0.44
2:O:372:ASP:CG	2:O:440:ARG:HG3	2.38	0.44
2:N:604:ILE:HG13	2:N:604:ILE:H	1.63	0.44
1:A:331:VAL:HG13	1:A:332:THR:N	2.32	0.44

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:626:MET:HB2	2:O:631:LEU:HD13	1.99	0.43
2:O:557:ILE:HD11	2:O:565:LYS:HB2	1.99	0.43
2:O:658:ILE:O	2:O:658:ILE:CG2	2.65	0.43
1:C:114:CYS:CA	11:C:1383:HOH:O	2.66	0.43
2:P:423:ARG:HH21	2:P:488:ARG:HH12	1.66	0.43
6:D:963:GOL:H2	2:P:27:HIS:CE1	2.54	0.43
1:B:200:THR:OG1	1:B:201:HIS:HD2	2.00	0.43
2:P:565:LYS:O	2:P:565:LYS:HD3	2.19	0.43
2:P:400:GLU:OE2	2:P:484:LYS:HE2	2.13	0.43
1:D:114:CYS:SG	1:D:209:HIS:CD2	3.12	0.43
1:A:118:ASN:OD1	1:A:209:HIS:HE1	2.01	0.43
1:C:284:ASN:HD22	1:C:285:PRO:N	2.17	0.43
1:B:284:ASN:C	1:B:284:ASN:HD22	2.21	0.43
2:O:383:PRO:HB2	2:O:474:VAL:HG21	2.01	0.43
2:P:400:GLU:OE1	2:P:484:LYS:HE3	2.18	0.43
2:P:342:MET:CG	2:P:384:LEU:HD22	2.40	0.43
1:A:550:CYS:CB	5:A:900:CYN:N	2.82	0.43
1:A:278:PHE:HB3	1:A:312:LEU:HD23	2.00	0.43
2:M:164:LYS:HD3	2:M:298:TYR:CE1	2.54	0.43
1:C:176:ARG:O	1:C:207:GLY:HA3	2.19	0.43
2:P:272:THR:HG22	2:P:272:THR:O	2.19	0.43
2:O:393:ARG:HG3	2:O:394:LYS:N	2.31	0.42
1:B:220:HIS:HD2	1:B:221:MET:O	2.01	0.42
2:O:353:VAL:HG22	2:O:388:VAL:HB	2.00	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:M:640[A]:GLN:HA	11:M:906:HOH:O	2.19	0.42
2:O:532:SER:H	2:O:535:ASP:HB2	1.84	0.42
2:P:471:GLU:HA	2:P:474:VAL:HG12	2.01	0.42
2:O:572:TYR:HA	2:O:579:LEU:O	2.18	0.42
2:P:541:GLU:H	2:P:541:GLU:HG2	1.63	0.42
2:P:448:LEU:O	2:P:452:MET:HG2	2.18	0.42
2:N:247:ARG:HD2	2:N:247:ARG:HA	1.82	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
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.33	0.42
1:C:615:LEU:HD23	1:C:615:LEU:O	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
2:N:384:LEU:HA	2:N:468:PHE:O	2.19	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:HG3	2:M:702:GLU:H	1.31	0.42
1:B:122:HIS:HD2	11:B:925:HOH:O	2.03	0.42
2:N:64:VAL:HG23	2:N:220:ASN:HB3	2.01	0.42
2:M:272:THR:O	2:M:272:THR:HG22	2.19	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: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
1:B:238:ALA:O	1:B:241:ASP:HB3	2.20	0.42
2:P:7:ILE:HD13	2:P:245:ARG:HG3	2.02	0.42
2:O:439:PHE:O	2:O:440:ARG:HD3	2.20	0.42
1:B:217:ASN:O	1:B:223:MET:HG3	2.19	0.42
2:N:247:ARG:HD2	2:N:247:ARG:N	2.32	0.42
1:C:98:VAL:HG13	1:C:610:VAL:HA	2.02	0.42
1:D:28:THR:OG1	1:D:477:GLN:NE2	2.53	0.42
1:D:128:ALA:HA	1:D:160:LEU:HD22	2.02	0.42
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.54	0.42
1:A:394:ILE:HG23	1:A:395:GLU:N	2.35	0.42
2:O:352:LEU:CD1	2:O:481:ALA:HA	2.47	0.42
2:N:353:VAL:HG22	2:N:388:VAL:HB	2.01	0.42
1:B:571:THR:N	1:B:572:PRO:CD	2.83	0.42
2:O:411:ILE:HG21	2:O:428:LEU:CD1	2.50	0.41
2:O:7:ILE:HD13	2:O:245:ARG:HD2	2.00	0.41
2:M:426:ASN:C	2:M:426:ASN:HD22	2.23	0.41
1:D:339:LEU:HD13	1:D:339:LEU:HA	1.87	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
1:D:414:SER:O	1:D:415:ASN:O	2.39	0.41
2:O:307:GLU:HG3	2:O:308:THR:N	2.34	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:395:MET:O	2:O:396:GLN:CB	2.67	0.41
2:O:347:THR:HA	2:O:348:PRO:HD2	1.82	0.41
2:O:431:SER:OG	2:O:434:ALA:HB2	2.20	0.41
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.84	0.41
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.55	0.41
2:N:262:LYS:HG3	11:N:2270:HOH:O	2.20	0.41
2:O:613:ILE:O	2:O:671:PRO:HD3	2.20	0.41
2:P:382:LEU:HG	2:P:469:THR:HB	2.02	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:A:529:LYS:HE2	11:A:1060:HOH:O	2.20	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
1:B:394:ILE:HG23	1:B:395:GLU:H	1.85	0.41
1:D:510:LEU:O	1:D:543:PRO:HD2	2.20	0.41
1:B:374:THR:HA	1:B:386:ILE:O	2.21	0.41
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.51	0.41
2:M:568:ASN:ND2	2:M:581:GLN:HE21	2.19	0.41
2:P:169:LEU:HG	2:P:193:LEU:HD21	2.02	0.41
2:O:505:SER:CB	2:O:570:TYR:HE2	2.33	0.41
2:P:602:MET:HE2	2:P:647:ILE:CG2	2.51	0.41
2:P:390:ILE:HD13	2:P:463:VAL:HG13	2.02	0.41
2:O:684:ARG:HH11	2:O:685:ARG:HG2	1.85	0.41
1:B:447:ASN:ND2	1:B:566:ASP:OD2	2.54	0.41
2:M:86:LYS:HD3	2:M:86:LYS:HA	1.83	0.41
1:D:496:VAL:HA	1:D:545:PHE:O	2.21	0.41
2:P:383:PRO:O	2:P:469:THR:HA	2.21	0.41
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.85	0.41
1:A:370:ARG:HG2	1:A:370:ARG:NH1	2.31	0.41
1:A:370:ARG:HH11	1:A:370:ARG:CG	2.33	0.41
2:M:383:PRO:HG2	2:M:469:THR:O	2.20	0.41
1:D:28:THR:HG21	1:D:33:VAL:HG12	2.02	0.41
2:P:496:THR:OG1	2:P:499:THR:HG23	2.20	0.41
1:B:483:THR:HB	1:B:638:PRO:HB2	2.02	0.41
2:M:122:LYS:HD2	2:M:125:GLU:OE1	2.20	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: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
2:N:204:TYR:CE1	2:N:331:GLU:HB2	2.56	0.40
2:P:701:ASP:N	2:P:704:ILE:HD13	2.36	0.40
2:P:219:ALA:O	2:P:223:LEU:HG	2.21	0.40
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.51	0.40
2:O:199:LYS:HZ2	2:O:199:LYS:HG3	1.51	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:720:HIS:HA	2:P:721:PRO:HD2	1.93	0.40
1:C:216:VAL:HG12	1:D:108:THR:HA	2.02	0.40
2:N:10:GLY:N	11:N:1249:HOH:O	2.28	0.40
2:P:358:GLU:O	2:P:359:SER:HB3	2.21	0.40
1:C:298:MET:HB3	1:C:298:MET:HE3	1.93	0.40
2:M:324:PHE:HA	2:M:413:TYR:O	2.22	0.40
1:A:105:MET:HB3	1:A:105:MET:HE3	1.91	0.40
2:P:342:MET:HB3	2:P:382:LEU:O	2.22	0.40
2:O:144:PHE:CE1	2:O:205:ILE:HG12	2.56	0.40
1:A:482:LEU:HA	1:A:482:LEU:HD22	1.90	0.40
2:N:721:PRO:O	2:N:725:MET:HG3	2.21	0.40
1:B:118:ASN:C	1:B:118:ASN:HD22	2.25	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
1:C:62:GLY:HA3	3:C:700:SF4:S4	2.61	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%)	46	42
1	B	678/673 (101%)	653 (96%)	23 (3%)	2 (0%)	46	42
1	C	674/673 (100%)	648 (96%)	25 (4%)	1 (0%)	56	57
1	D	671/673 (100%)	645 (96%)	22 (3%)	4 (1%)	30	21
2	M	730/728 (100%)	697 (96%)	28 (4%)	5 (1%)	26	18
2	N	727/728 (100%)	700 (96%)	22 (3%)	5 (1%)	26	18
2	O	727/728 (100%)	650 (89%)	51 (7%)	26 (4%)	4	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	P	728/728 (100%)	684 (94%)	37 (5%)	7 (1%)	19 11
All	All	5611/5604 (100%)	5328 (95%)	231 (4%)	52 (1%)	21 13

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 (i)

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%)	47 47
1	B	549/542 (101%)	534 (97%)	15 (3%)	52 53
1	C	543/542 (100%)	530 (98%)	13 (2%)	57 60
1	D	541/542 (100%)	529 (98%)	12 (2%)	60 63
2	M	614/610 (101%)	581 (95%)	33 (5%)	27 22
2	N	611/610 (100%)	571 (94%)	40 (6%)	21 15
2	O	611/610 (100%)	540 (88%)	71 (12%)	7 3
2	P	612/610 (100%)	557 (91%)	55 (9%)	12 6
All	All	4628/4608 (100%)	4372 (94%)	256 (6%)	27 21

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	A	700	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	A	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	A	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	A	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	A	963	-	5,5,5	0.66	0	5,5,5	1.69	1 (20%)
3	SF4	B	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	B	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	B	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	B	963	-	5,5,5	0.80	0	5,5,5	1.59	1 (20%)
3	SF4	C	700	1	0,12,12	0.00	-	0,24,24	0.00	-
3	SF4	C	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	C	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	CYN	C	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	C	963	-	5,5,5	0.55	0	5,5,5	0.89	0
3	SF4	D	750	1	0,12,12	0.00	-	0,24,24	0.00	-
4	XCC	D	800	1,11	0,11,11	0.00	-	0,19,19	0.00	-
5	CYN	D	900	-	0,1,1	0.00	-	0,0,0	0.00	-
6	GOL	D	963	-	5,5,5	0.71	0	5,5,5	1.31	1 (20%)
3	SF4	M	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	M	953	-	2,2,3	0.77	0	0,1,3	0.00	-
3	SF4	N	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	N	953	-	2,2,3	0.83	0	0,1,3	0.00	-
3	SF4	O	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	O	953	-	2,2,3	0.83	0	0,1,3	0.00	-
3	SF4	P	900	2	0,12,12	0.00	-	0,24,24	0.00	-
9	ACT	P	953	-	2,2,3	0.86	0	0,1,3	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	A	700	1	-	0/0/48/48	0/6/5/5
3	SF4	A	750	1	-	0/0/48/48	0/6/5/5
4	XCC	A	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	A	900	-	-	0/0/0/0	0/0/0/0
6	GOL	A	963	-	-	0/4/4/4	0/0/0/0
3	SF4	B	750	1	-	0/0/48/48	0/6/5/5
4	XCC	B	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	B	900	-	-	0/0/0/0	0/0/0/0
6	GOL	B	963	-	-	0/4/4/4	0/0/0/0
3	SF4	C	700	1	-	0/0/48/48	0/6/5/5
3	SF4	C	750	1	-	0/0/48/48	0/6/5/5
4	XCC	C	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	C	900	-	-	0/0/0/0	0/0/0/0
6	GOL	C	963	-	-	0/4/4/4	0/0/0/0
3	SF4	D	750	1	-	0/0/48/48	0/6/5/5
4	XCC	D	800	1,11	-	0/0/32/32	0/0/3/3
5	CYN	D	900	-	-	0/0/0/0	0/0/0/0
6	GOL	D	963	-	-	0/4/4/4	0/0/0/0
3	SF4	M	900	2	-	0/0/48/48	0/6/5/5
9	ACT	M	953	-	-	0/0/0/0	0/0/0/0
3	SF4	N	900	2	-	0/0/48/48	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ACT	N	953	-	-	0/0/0/0	0/0/0/0
3	SF4	O	900	2	-	0/0/48/48	0/6/5/5
9	ACT	O	953	-	-	0/0/0/0	0/0/0/0
3	SF4	P	900	2	-	0/0/48/48	0/6/5/5
9	ACT	P	953	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	963	GOL	O1-C1-C2	-2.29	99.10	110.18
6	A	963	GOL	O1-C1-C2	-2.26	99.24	110.18
6	B	963	GOL	O2-C2-C3	-2.21	98.50	108.65

There are no chirality outliers.

There are no torsion outliers.

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
6	A	963	GOL	1	0
3	C	700	SF4	1	0
5	C	900	CYN	3	0
6	C	963	GOL	4	0
5	D	900	CYN	1	0
6	D	963	GOL	6	0
9	M	953	ACT	1	0
9	N	953	ACT	3	0
9	O	953	ACT	1	0
9	P	953	ACT	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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	673/673 (100%)	0.03	40 (5%) 26 36	14, 24, 42, 62	0
1	B	673/673 (100%)	-0.01	27 (4%) 42 52	14, 22, 39, 66	0
1	C	673/673 (100%)	-0.17	16 (2%) 62 71	18, 26, 41, 57	0
1	D	673/673 (100%)	0.01	26 (3%) 43 54	19, 28, 43, 62	0
2	M	728/728 (100%)	-0.02	21 (2%) 55 65	16, 31, 58, 76	0
2	N	728/728 (100%)	0.04	24 (3%) 50 60	16, 30, 57, 71	0
2	O	728/728 (100%)	2.11	326 (44%) 0 1	25, 62, 88, 123	0
2	P	728/728 (100%)	0.86	159 (21%) 1 2	19, 45, 79, 107	0
All	All	5604/5604 (100%)	0.37	639 (11%) 7 11	14, 29, 74, 123	0

All (639) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	481	ALA	14.6
2	O	486	LYS	10.0
2	O	490	ASP	9.9
2	O	474	VAL	9.9
2	O	485	TYR	9.9
2	O	380	SER	9.7
2	O	494	GLY	9.6
2	O	361	ILE	9.4
2	O	461	ASP	9.4
2	O	493	ARG	9.2
2	O	728	ILE	8.7
2	O	340	VAL	8.6
2	O	381	LYS	8.6
2	O	357	SER	8.2
2	O	567	VAL	8.2
2	P	461	ASP	8.2

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Mol	Chain	Res	Type	RSRZ
2	O	712	LEU	8.2
2	O	339	TYR	8.1
2	O	476	GLU	8.0
2	P	483	GLU	8.0
2	O	658	ILE	7.8
2	O	724	THR	7.8
2	P	391	TYR	7.7
2	O	391	TYR	7.7
2	O	564	TRP	7.6
2	O	470	ASP	7.6
2	O	458	ALA	7.6
2	O	369	ILE	7.5
2	O	399	PHE	7.5
2	P	485	TYR	7.5
2	O	450	ALA	7.4
2	O	729	MET	7.3
2	O	653	VAL	7.2
2	O	390	ILE	7.2
2	O	384	LEU	7.2
2	O	333	ILE	7.1
2	O	696	ILE	7.1
2	O	542	ILE	7.0
2	O	359	SER	7.0
2	O	468	PHE	7.0
2	O	492	MET	7.0
2	O	725	MET	6.9
2	P	728	ILE	6.9
2	O	397	ALA	6.9
2	O	356	VAL	6.8
2	O	560	ILE	6.8
2	O	407	ILE	6.7
2	O	379	GLY	6.7
2	O	342	MET	6.7
2	O	316	ILE	6.6
2	O	373	ILE	6.6
2	O	424	ASN	6.6
2	O	704	ILE	6.5
2	O	478	MET	6.5
2	O	574	ALA	6.5
2	P	487	GLU	6.5
2	O	348	PRO	6.5
2	O	691	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
2	O	376	ILE	6.4
2	O	472	ALA	6.4
2	O	456	PHE	6.4
2	O	479	GLU	6.3
2	O	449	VAL	6.3
2	O	683	VAL	6.3
2	O	427	TRP	6.3
2	O	559	PRO	6.3
2	P	356	VAL	6.3
2	O	718	LYS	6.2
2	P	491	ARG	6.2
2	P	481	ALA	6.2
2	O	664	ILE	6.2
2	O	699	ILE	6.2
2	P	361	ILE	6.1
1	D	417	PRO	6.1
2	P	393	ARG	6.1
2	O	354	ARG	6.0
2	O	439	PHE	5.9
2	O	368	VAL	5.9
2	O	570	TYR	5.8
2	P	552	PRO	5.8
2	O	695	PHE	5.8
2	O	418	TRP	5.8
2	P	729	MET	5.8
2	O	488	ARG	5.7
2	O	566	SER	5.7
2	O	714	TYR	5.7
2	O	483	GLU	5.7
2	P	355	THR	5.6
2	O	463	VAL	5.6
2	O	462	ARG	5.6
2	O	392	GLY	5.6
2	P	369	ILE	5.6
2	O	398	ASP	5.6
2	O	362	THR	5.6
2	O	469	THR	5.5
2	P	359	SER	5.5
2	O	657	PHE	5.5
2	O	722	ALA	5.5
2	O	690	GLY	5.5
2	O	665	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
2	O	363	ASP	5.5
2	P	348	PRO	5.4
2	O	435	VAL	5.4
2	O	460	VAL	5.4
2	P	493	ARG	5.3
2	O	540	TYR	5.3
2	O	422	GLN	5.3
2	O	347	THR	5.3
2	O	489	ASP	5.3
2	O	353	VAL	5.3
1	D	416	ARG	5.3
2	O	364	GLY	5.2
2	O	389	ASP	5.2
2	P	492	MET	5.2
2	O	350	PHE	5.2
2	O	579	LEU	5.2
2	O	495	LEU	5.2
2	O	14	GLU	5.2
2	O	668	VAL	5.1
2	O	504	TYR	5.1
1	A	107	LEU	5.1
2	P	490	ASP	5.0
2	O	314	THR	5.0
2	O	484	LYS	5.0
2	O	685	ARG	5.0
2	O	436	ALA	5.0
2	P	364	GLY	5.0
2	P	458	ALA	5.0
2	O	366	ILE	5.0
2	O	727	PRO	5.0
2	O	623	PRO	4.9
2	O	584	LEU	4.9
2	O	697	ASP	4.9
2	O	491	ARG	4.9
2	O	387	LEU	4.9
2	O	425	ILE	4.9
2	O	365	LYS	4.9
2	P	472	ALA	4.9
2	O	533	TRP	4.9
2	O	717	GLU	4.9
2	O	663	GLY	4.9
2	N	729	MET	4.8

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Mol	Chain	Res	Type	RSRZ
2	O	692	GLY	4.8
2	O	723	LEU	4.8
2	O	667	ILE	4.8
2	O	465	VAL	4.8
2	O	573	THR	4.8
2	O	426	ASN	4.7
2	P	704	ILE	4.7
2	P	712	LEU	4.7
2	P	542	ILE	4.7
2	P	474	VAL	4.7
2	P	682	PHE	4.7
2	O	423	ARG	4.7
2	P	572	TYR	4.6
2	O	541	GLU	4.6
2	O	440	ARG	4.6
2	O	715	LEU	4.6
1	A	106	ILE	4.6
2	O	6	LYS	4.6
2	O	694	ASP	4.6
2	P	358	GLU	4.6
2	O	451	LYS	4.6
2	P	392	GLY	4.6
2	O	611	ILE	4.6
2	O	475	LYS	4.6
2	O	684	ARG	4.6
2	O	713	PRO	4.5
2	O	375	GLN	4.5
2	O	343	GLY	4.5
2	P	314	THR	4.5
2	P	362	THR	4.5
2	O	608	CYS	4.5
2	O	377	PRO	4.5
2	O	693	GLU	4.5
2	P	368	VAL	4.5
2	P	354	ARG	4.5
2	O	355	THR	4.4
1	A	104[A]	LEU	4.4
2	O	545	ALA	4.4
2	O	666	ARG	4.4
2	P	696	ILE	4.4
2	P	363	ASP	4.4
2	O	716	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
2	P	390	ILE	4.4
2	O	401	GLY	4.4
2	O	719	GLY	4.4
2	O	703	THR	4.4
2	O	583	CYS	4.3
2	P	623	PRO	4.3
2	O	467	ILE	4.3
2	O	612	MET	4.3
2	O	655	LYS	4.3
2	P	425	ILE	4.3
2	P	694	ASP	4.3
2	O	679	HIS	4.3
2	O	651	TYR	4.3
2	M	314	THR	4.2
2	O	534	LEU	4.2
2	O	400	GLU	4.2
2	O	344	GLY	4.2
2	M	316	ILE	4.2
2	O	457	PRO	4.2
2	P	402	VAL	4.2
1	B	107	LEU	4.2
2	O	543	ASN	4.2
2	O	586	THR	4.1
2	P	462	ARG	4.1
2	O	319	ASP	4.1
1	D	415	ASN	4.1
2	P	690	GLY	4.1
2	O	698	LYS	4.1
2	M	729	MET	4.1
2	O	334	ARG	4.1
2	O	471	GLU	4.1
2	M	318	LEU	4.1
2	O	563	ILE	4.1
2	O	502	THR	4.1
2	O	674	LEU	4.0
2	O	395	MET	4.0
2	O	519	ILE	4.0
2	O	613	ILE	4.0
2	O	678	LEU	4.0
2	P	476	GLU	4.0
2	O	336	GLY	4.0
2	O	726	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	O	393	ARG	4.0
2	P	14	GLU	4.0
2	P	692	GLY	3.9
1	A	415	ASN	3.9
2	O	605	LEU	3.9
2	O	522	PRO	3.9
2	O	428	LEU	3.9
2	P	427	TRP	3.9
2	O	551	ILE	3.9
1	B	539	ILE	3.8
2	P	334	ARG	3.8
2	P	486	LYS	3.8
2	O	554	GLU	3.8
2	O	552	PRO	3.8
2	O	352	LEU	3.8
2	O	631	LEU	3.8
2	P	15	GLY	3.8
1	C	104	LEU	3.8
2	O	670	MET	3.8
2	P	494	GLY	3.8
2	O	711	ILE	3.7
2	P	560	ILE	3.7
2	P	570	TYR	3.7
2	O	606	PRO	3.7
2	O	686	SER	3.7
2	O	480	VAL	3.7
2	P	460	VAL	3.7
2	P	714	TYR	3.7
2	P	470	ASP	3.7
2	O	317	LYS	3.7
2	O	635	ILE	3.7
2	O	682	PHE	3.6
2	N	373	ILE	3.6
2	O	358	GLU	3.6
2	O	338	MET	3.6
1	A	216	VAL	3.6
2	O	708	VAL	3.6
2	O	466	THR	3.6
2	P	475	LYS	3.6
2	O	582	VAL	3.6
2	O	360	GLU	3.6
1	D	104	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	O	477	TYR	3.6
2	O	555	GLY	3.6
2	O	374	ASP	3.6
2	O	587	LEU	3.5
2	O	580	GLU	3.5
2	O	520	VAL	3.5
2	O	442	LYS	3.5
2	P	387	LEU	3.5
2	O	650	THR	3.5
2	O	394	LYS	3.5
2	O	669	TRP	3.5
2	O	621	MET	3.5
2	O	577	ARG	3.5
2	O	645	MET	3.5
2	O	498	GLU	3.5
2	O	707	THR	3.5
2	P	423	ARG	3.5
2	O	388	VAL	3.5
2	P	367	GLU	3.5
2	O	15	GLY	3.5
2	P	340	VAL	3.4
2	O	367	GLU	3.4
2	O	482	ARG	3.4
2	P	718	LYS	3.4
1	B	104[A]	LEU	3.4
1	C	230	LEU	3.4
2	P	403	LEU	3.4
2	O	572	TYR	3.4
2	O	687	VAL	3.4
2	O	721	PRO	3.4
2	P	703	THR	3.4
1	C	215	LEU	3.4
2	O	571	LEU	3.4
1	C	106	ILE	3.4
2	O	585	TYR	3.4
2	P	477	TYR	3.4
2	P	719	GLY	3.4
2	P	684[A]	ARG	3.4
2	P	724	THR	3.3
2	P	353	VAL	3.3
2	O	550	PRO	3.3
2	O	453	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	O	565	LYS	3.3
2	O	349	ALA	3.3
1	B	106	ILE	3.3
2	O	383	PRO	3.3
1	B	216	VAL	3.3
2	O	385	GLY	3.3
2	P	711	ILE	3.3
2	O	709	ASP	3.3
1	B	537	ILE	3.3
2	O	3	ASP	3.3
2	O	9	GLU	3.3
1	A	108	THR	3.3
2	O	671	PRO	3.3
2	O	652	ILE	3.2
2	O	581	GLN	3.2
2	O	659	SER	3.2
1	D	215	LEU	3.2
2	P	374	ASP	3.2
2	P	467	ILE	3.2
1	C	216	VAL	3.2
2	O	517	VAL	3.2
2	P	399	PHE	3.2
2	P	468	PHE	3.2
2	P	544	HIS	3.2
2	P	727	PRO	3.2
1	A	231	VAL	3.2
2	N	314	THR	3.2
2	O	625	GLY	3.2
1	B	219	ALA	3.2
2	O	351	GLU	3.2
2	P	698	LYS	3.2
2	O	372	ASP	3.2
2	O	609	ASN	3.2
2	O	662	GLY	3.2
1	B	538	GLU	3.2
2	O	487	GLU	3.2
2	P	707	THR	3.2
2	N	318	LEU	3.2
2	N	468	PHE	3.2
2	O	382	LEU	3.2
2	P	715	LEU	3.2
2	O	447	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
2	O	544	HIS	3.1
1	A	230	LEU	3.1
2	P	350	PHE	3.1
2	O	464	GLN	3.1
2	O	370	GLY	3.1
2	P	695	PHE	3.1
2	P	284	GLU	3.1
2	P	124	ASP	3.1
1	B	215	LEU	3.0
2	P	687	VAL	3.0
2	P	565	LYS	3.0
2	O	720	HIS	3.0
1	B	536	ASN	3.0
2	O	341	GLU	3.0
2	P	660	ALA	3.0
2	O	124	ASP	3.0
2	P	488	ARG	3.0
2	O	689	GLU	3.0
2	O	459	ILE	3.0
2	N	346	ARG	3.0
2	O	332	SER	3.0
2	M	14	GLU	3.0
2	N	316	ILE	3.0
2	P	424	ASN	3.0
2	P	377	PRO	3.0
1	A	215	LEU	2.9
2	O	318	LEU	2.9
2	N	348	PRO	2.9
2	O	335	LYS	2.9
2	O	496	THR	2.9
2	P	484	LYS	2.9
2	O	700	ALA	2.9
2	P	721	PRO	2.9
1	B	212	ILE	2.9
2	P	566	SER	2.9
2	P	567	VAL	2.9
2	M	472	ALA	2.9
2	O	345	ASN	2.9
2	O	378	GLU	2.9
2	O	681	GLU	2.9
2	O	295	VAL	2.9
2	O	614	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	622	THR	2.9
2	P	432	LYS	2.9
1	A	416	ARG	2.9
1	C	107	LEU	2.9
2	P	16	LYS	2.9
1	B	231	VAL	2.9
1	D	216	VAL	2.9
2	P	722	ALA	2.9
2	M	470	ASP	2.9
2	O	2	THR	2.9
2	O	396	GLN	2.8
1	A	70	PHE	2.8
2	O	656	LYS	2.8
1	A	103	GLY	2.8
1	A	619	ILE	2.8
1	D	107	LEU	2.8
2	O	526	GLY	2.8
2	O	433	ASP	2.8
2	P	335	LYS	2.8
2	N	470	ASP	2.8
2	O	639	THR	2.8
2	P	580	GLU	2.8
1	B	70	PHE	2.7
1	A	590	ALA	2.7
2	O	371	PRO	2.7
2	P	541	GLU	2.7
2	O	705	GLY	2.7
1	C	231	VAL	2.7
2	O	402	VAL	2.7
2	O	443	ASN	2.7
2	N	472	ALA	2.7
2	O	499	THR	2.7
1	D	368	HIS	2.7
2	O	640	GLN	2.7
1	B	591	ILE	2.7
2	O	672	LYS	2.7
1	C	109	GLY	2.7
2	O	151	TRP	2.7
2	P	610	GLY	2.7
1	D	304	ALA	2.7
2	N	381	LYS	2.7
2	P	357	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	O	710	GLU	2.7
2	P	400	GLU	2.7
2	P	555	GLY	2.7
2	P	333	ILE	2.6
2	O	702	GLU	2.6
2	P	479	GLU	2.6
2	P	533	TRP	2.6
2	O	432	LYS	2.6
2	M	693	GLU	2.6
1	A	228	VAL	2.6
2	O	507	VAL	2.6
2	P	473	LYS	2.6
1	A	212	ILE	2.6
1	A	234	ALA	2.6
2	O	680	ASP	2.6
2	P	697	ASP	2.6
2	N	475	LYS	2.6
2	M	124	ASP	2.6
2	P	13	PRO	2.6
1	B	234	ALA	2.6
1	D	589	ALA	2.6
2	P	480	VAL	2.6
1	A	105	MET	2.6
2	O	16	LYS	2.6
2	O	410	PHE	2.6
2	O	501	ASP	2.6
1	B	230	LEU	2.6
2	O	313	LEU	2.6
2	P	395	MET	2.6
2	P	471	GLU	2.6
2	N	474	VAL	2.6
2	O	13	PRO	2.5
2	O	503	PHE	2.5
2	P	606	PRO	2.5
2	M	469	THR	2.5
2	N	367	GLU	2.5
2	P	668	VAL	2.5
2	O	321	PRO	2.5
2	O	641	THR	2.5
1	D	588	ALA	2.5
2	P	577	ARG	2.5
1	B	590	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	102	VAL	2.5
1	C	102	VAL	2.5
1	D	106	ILE	2.5
2	O	289	PRO	2.5
1	B	108	THR	2.5
2	M	719	GLY	2.5
2	P	554	GLU	2.5
2	O	429	ARG	2.5
2	P	503	PHE	2.5
1	A	109	GLY	2.5
2	P	501	ASP	2.5
2	O	576	ASN	2.4
2	O	602	MET	2.4
2	P	665	ALA	2.4
2	P	661	ASP	2.4
1	A	589	ALA	2.4
2	P	693	GLU	2.4
2	P	573	THR	2.4
2	P	376	ILE	2.4
2	P	381	LYS	2.4
2	O	569	ASP	2.4
2	P	569	ASP	2.4
2	P	394	LYS	2.4
2	O	592	MET	2.4
1	A	237	VAL	2.4
2	O	416	GLY	2.4
1	B	112	ALA	2.4
1	C	227	PRO	2.4
2	O	454	GLU	2.4
2	P	581	GLN	2.4
2	P	584	LEU	2.4
2	O	610	GLY	2.4
2	O	11	ALA	2.4
1	A	591	ILE	2.4
2	M	713	PRO	2.4
2	P	688	GLU	2.4
2	P	375	GLN	2.4
2	O	421	GLY	2.4
2	P	384	LEU	2.4
2	P	469	THR	2.4
2	O	548	ASN	2.4
1	C	590	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	642	PRO	2.3
1	D	235	ILE	2.3
2	P	553	LYS	2.3
2	P	382	LEU	2.3
2	O	677	PHE	2.3
2	P	418	TRP	2.3
1	D	591	ILE	2.3
2	O	557	ILE	2.3
2	P	551	ILE	2.3
2	N	339	TYR	2.3
1	B	110	ALA	2.3
1	D	590	ALA	2.3
2	O	530	ALA	2.3
2	O	430	VAL	2.3
2	O	647	ILE	2.3
2	O	661	ASP	2.3
1	D	108	THR	2.3
2	O	508	LEU	2.3
1	A	110	ALA	2.3
2	N	391	TYR	2.3
1	B	103	GLY	2.3
2	M	345	ASN	2.3
2	P	389	ASP	2.3
1	D	231	VAL	2.3
2	M	369	ILE	2.3
2	O	634	MET	2.3
2	N	11	ALA	2.3
2	O	549	GLN	2.3
2	P	6	LYS	2.3
1	D	596	VAL	2.3
2	N	469	THR	2.3
1	D	413	GLU	2.3
1	C	219	ALA	2.3
2	N	145	GLY	2.2
2	M	348	PRO	2.2
2	O	556	GLU	2.2
2	M	696	ILE	2.2
2	P	701	ASP	2.2
1	A	219	ALA	2.2
2	O	594	SER	2.2
2	M	16	LYS	2.2
1	A	235	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	664	ILE	2.2
2	M	317	LYS	2.2
2	P	622	THR	2.2
2	N	141	VAL	2.2
1	A	99	ALA	2.2
1	B	71	CYS	2.2
2	O	688	GLU	2.2
1	C	70	PHE	2.2
2	O	558	ASP	2.2
2	O	676	ASP	2.2
1	D	212	ILE	2.2
2	M	381	LYS	2.2
1	A	620	LEU	2.2
2	O	246	ARG	2.2
1	A	534	GLY	2.2
2	P	708	VAL	2.2
2	P	365	LYS	2.2
1	B	619	ILE	2.2
2	P	457	PRO	2.2
1	B	233	SER	2.1
1	D	103	GLY	2.1
2	N	360	GLU	2.1
2	N	564	TRP	2.1
1	A	111	ALA	2.1
2	O	660	ALA	2.1
2	O	604	ILE	2.1
2	O	561	LYS	2.1
2	P	583	CYS	2.1
2	P	482	ARG	2.1
1	C	228	VAL	2.1
2	O	588	MET	2.1
2	P	680	ASP	2.1
1	B	109	GLY	2.1
2	O	654	SER	2.1
2	O	675	LYS	2.1
2	M	339	TYR	2.1
1	B	627	VAL	2.1
2	P	435	VAL	2.1
2	O	431	SER	2.1
2	N	440	ARG	2.1
2	O	538	ALA	2.1
1	A	232	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	98	VAL	2.1
1	D	353	VAL	2.1
2	O	287	GLN	2.1
2	O	437	LYS	2.1
1	A	96	THR	2.1
1	C	616	ILE	2.1
2	O	403	LEU	2.1
1	D	155	GLU	2.1
2	M	284	GLU	2.1
1	A	148	ARG	2.1
1	B	589	ALA	2.1
2	O	405	ARG	2.1
2	P	343	GLY	2.1
2	P	349	ALA	2.1
2	O	575	SER	2.1
1	D	232	PHE	2.1
1	A	596	VAL	2.1
1	D	355	CYS	2.1
2	P	398	ASP	2.1
2	P	366	ILE	2.0
2	P	371	PRO	2.0
1	A	112	ALA	2.0
1	A	223	MET	2.0
2	P	675	LYS	2.0
1	A	71	CYS	2.0
2	O	7	ILE	2.0
2	P	586	THR	2.0
1	A	608	PRO	2.0
2	P	713	PRO	2.0
1	A	114[A]	CYS	2.0
2	N	370	GLY	2.0
2	P	341	GLU	2.0
1	A	585	SER	2.0
1	D	539	ILE	2.0
2	P	459	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	ACT	P	953	3/4	0.87	0.51	22.18	75,75,76,76	0
9	ACT	O	953	3/4	0.85	0.41	7.42	109,109,109,109	0
5	CYN	C	900	2/2	0.93	0.28	3.37	31,31,31,33	0
6	GOL	B	963	6/6	0.90	0.18	3.07	27,37,38,44	0
9	ACT	M	953	3/4	0.95	0.23	2.62	55,55,56,56	0
9	ACT	N	953	3/4	0.92	0.23	2.04	71,71,71,71	0
6	GOL	C	963	6/6	0.91	0.20	1.91	50,53,54,55	0
6	GOL	A	963	6/6	0.90	0.18	1.58	26,30,37,38	0
10	NA	P	730	1/1	0.88	0.14	0.59	35,35,35,35	0
6	GOL	D	963	6/6	0.93	0.13	0.52	38,43,45,45	0
3	SF4	D	750	8/8	0.99	0.13	-0.29	24,24,26,26	0
3	SF4	M	900	8/8	0.99	0.11	-0.53	20,22,23,23	0
4	XCC	D	800	9/9	0.99	0.12	-0.65	27,30,36,36	0
4	XCC	C	800	9/9	0.99	0.11	-0.65	19,25,28,31	0
3	SF4	C	750	8/8	0.99	0.10	-0.69	26,27,28,29	0
3	SF4	A	750	8/8	1.00	0.13	-0.71	17,17,18,19	0
3	SF4	N	900	8/8	0.99	0.11	-0.78	20,23,24,25	0
3	SF4	C	700	8/8	0.99	0.09	-0.80	24,29,31,31	0
3	SF4	B	750	8/8	0.99	0.12	-0.88	16,16,18,18	0
4	XCC	A	800	9/9	0.99	0.13	-0.89	21,22,25,26	0
10	NA	N	730	1/1	0.94	0.08	-0.93	26,26,26,26	0
3	SF4	A	700	8/8	0.99	0.09	-1.04	16,17,19,20	0
5	CYN	A	900	2/2	0.94	0.17	-1.13	31,31,31,32	0
4	XCC	B	800	9/9	0.99	0.12	-1.15	18,19,24,26	0
7	CU1	M	950	1/1	0.99	0.09	-1.15	35,35,35,35	0
10	NA	O	730	1/1	0.76	0.07	-1.37	64,64,64,64	0
3	SF4	P	900	8/8	0.99	0.05	-1.49	38,41,42,42	0
8	NI	N	951	1/1	1.00	0.10	-1.49	24,24,24,24	0
5	CYN	B	900	2/2	0.94	0.13	-1.57	25,25,25,25	0
8	NI	M	951	1/1	1.00	0.10	-1.70	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	CYN	D	900	2/2	0.98	0.13	-2.10	42,42,42,43	0
3	SF4	O	900	8/8	0.93	0.06	-2.13	57,60,62,64	0
7	CU1	N	950	1/1	0.99	0.09	-2.32	34,34,34,34	0
8	NI	P	951	1/1	0.99	0.04	-2.55	41,41,41,41	0
7	CU1	P	950	1/1	0.98	0.03	-2.56	49,49,49,49	0
7	CU1	O	950	1/1	0.98	0.03	-3.31	73,73,73,73	0
10	NA	M	1	1/1	0.97	0.07	-3.38	28,28,28,28	0
8	NI	O	951	1/1	0.97	0.04	-3.78	66,66,66,66	0

6.5 Other polymers

There are no such residues in this entry.