



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:20 pm BST

PDB ID : 2Z8Y  
Title : Xenon-bound structure of bifunctional carbon monoxide dehydrogenase/acet  
yl-CoA synthase(CODH/ACS) from Moorella thermoacetica  
Authors : Doukov, T.I.; Blasiak, L.C.; Drennan, C.L.  
Deposited on : 2007-09-12  
Resolution : 2.51 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.

---

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

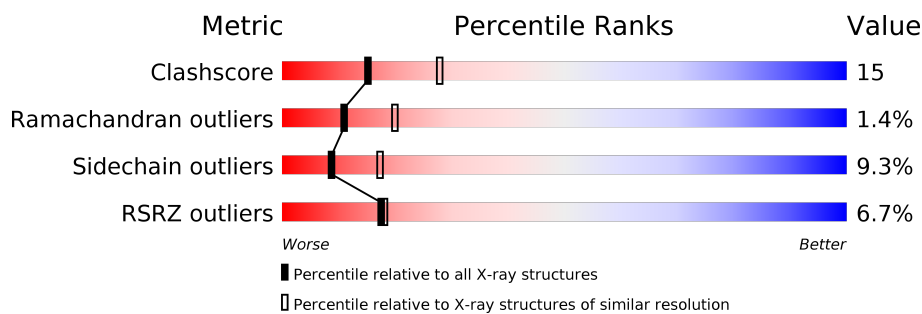
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	674	<div> <div>2%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	B	674	<div> <div>%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	C	674	<div> <div>%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	D	674	<div> <div>2%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	M	729	<div> <div>%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
2	N	729	<div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	O	729	<div> <div>30%</div> <div>45%</div> <div>43%</div> <div>11%</div> <div>.</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	P	729	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	O	900	-	-	X	-
4	XCC	A	800	-	-	X	-
4	XCC	B	800	-	-	X	-
4	XCC	C	800	-	-	X	-
5	XE	A	1001	-	-	X	-
5	XE	A	1003[A]	-	-	X	-
5	XE	A	1003[B]	-	-	X	-
5	XE	A	1004	-	-	X	-
5	XE	B	1001	-	-	X	-
5	XE	B	1003[B]	-	-	X	-
5	XE	B	1004	-	-	X	-
5	XE	C	1003[B]	-	-	X	-
5	XE	C	1004	-	-	X	-
5	XE	D	1003[B]	-	-	X	-
5	XE	M	1006	-	-	X	-
5	XE	N	1006	-	-	X	-
5	XE	N	1009	-	-	X	-
5	XE	O	1006	-	-	X	-
5	XE	O	1009	-	-	X	-
5	XE	P	1008	-	-	X	-
6	GOL	D	863	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 44706 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.

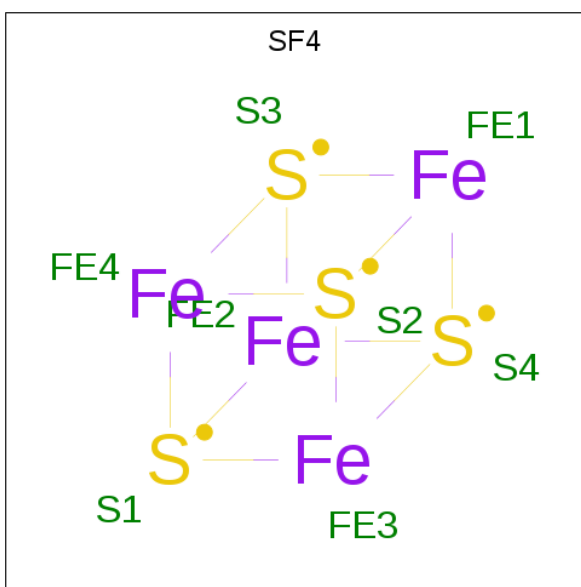
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total	C	N	O	S	0	2	0
			5094	3202	891	959	42			
1	B	673	Total	C	N	O	S	0	7	0
			5094	3202	891	959	42			
1	C	673	Total	C	N	O	S	0	4	0
			5094	3202	891	959	42			
1	D	673	Total	C	N	O	S	0	2	0
			5094	3202	891	959	42			

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

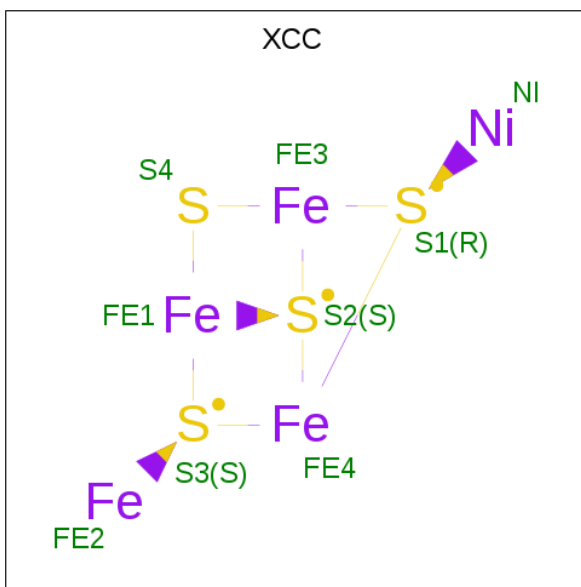
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5740	3681	956	1068	35			
2	N	728	Total	C	N	O	S	0	3	0
			5740	3681	956	1068	35			
2	O	727	Total	C	N	O	S	0	1	0
			5725	3673	952	1066	34			
2	P	728	Total	C	N	O	S	0	3	0
			5740	3681	956	1068	35			

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



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

- Molecule 4 is FE(4)-NI(1)-S(4) CLUSTER (three-letter code: XCC) (formula: Fe<sub>4</sub>NiS<sub>4</sub>).



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

- Molecule 5 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	4	Total	Xe	0	0
			4	4		
5	D	6	Total	Xe	0	1
			7	7		
5	B	6	Total	Xe	0	1
			7	7		
5	C	6	Total	Xe	0	1
			7	7		
5	A	6	Total	Xe	0	1
			7	7		
5	N	4	Total	Xe	0	0
			4	4		
5	O	3	Total	Xe	0	0
			3	3		
5	M	3	Total	Xe	0	0
			3	3		

- 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	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- 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
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 water.

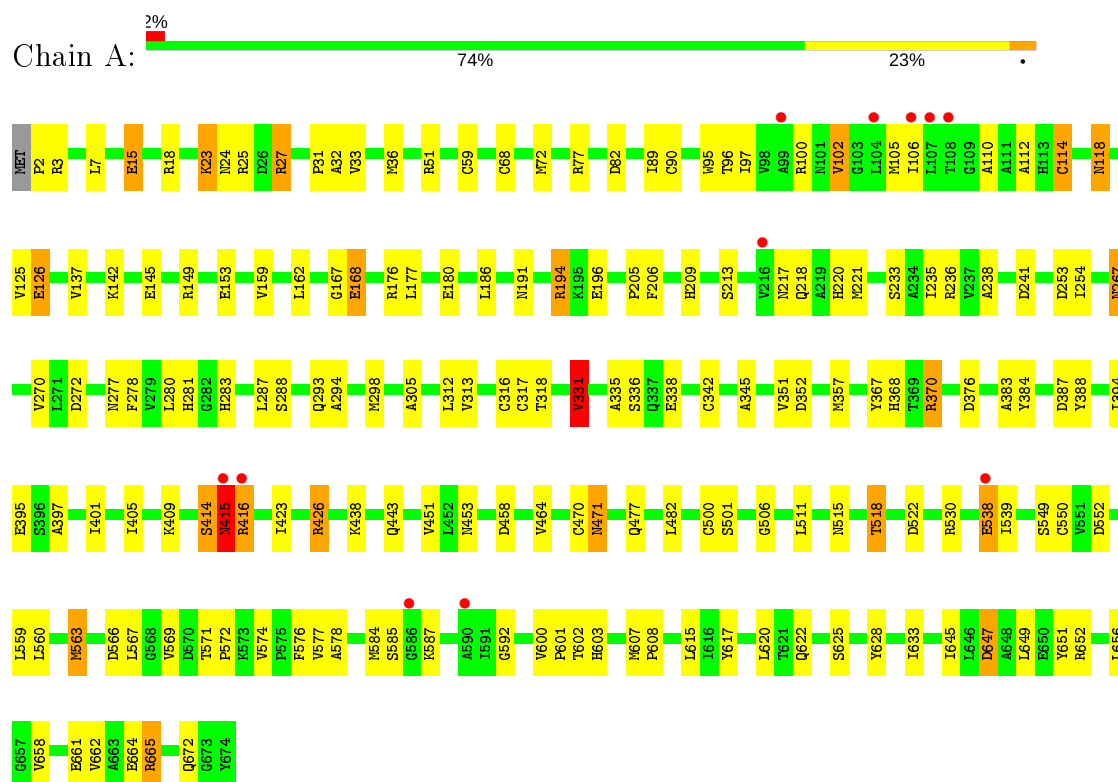
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	168	Total O 168 168	0	0
9	B	220	Total O 220 220	0	0
9	C	130	Total O 130 130	0	0
9	D	105	Total O 105 105	0	0
9	M	201	Total O 201 201	0	0
9	N	222	Total O 222 222	0	0
9	O	27	Total O 27 27	0	0
9	P	80	Total O 80 80	0	0



### 3 Residue-property plots

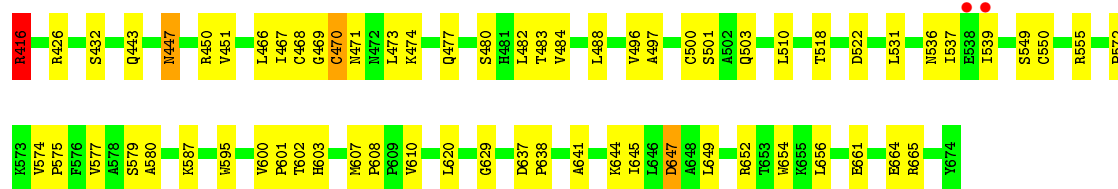
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

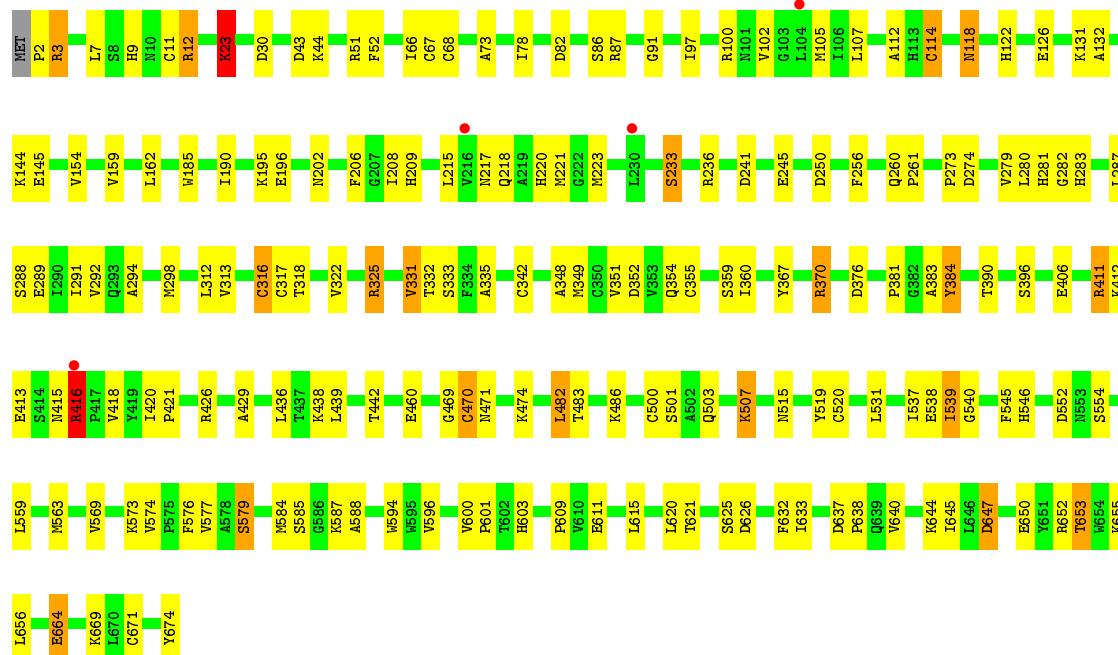


- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

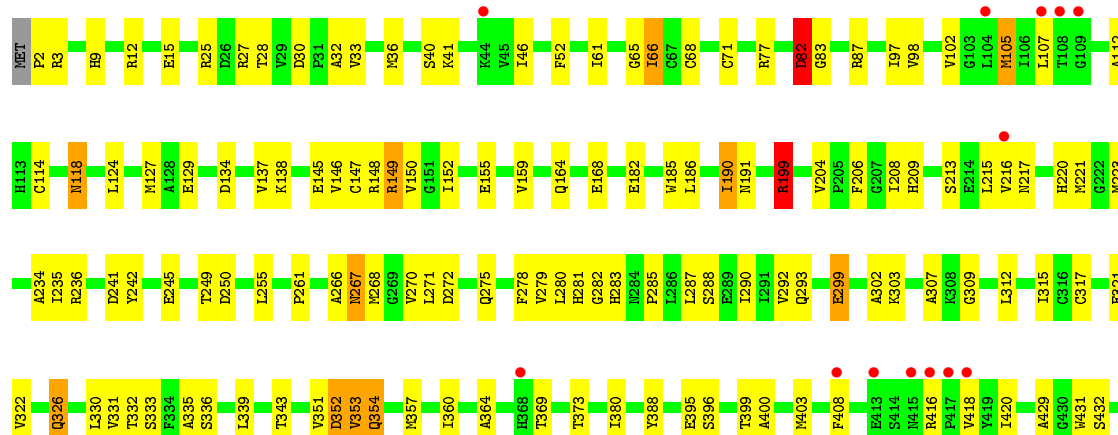


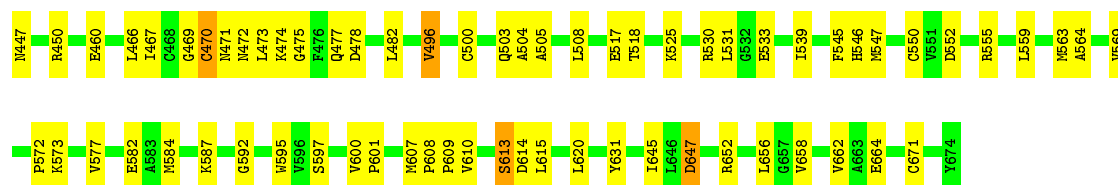


- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

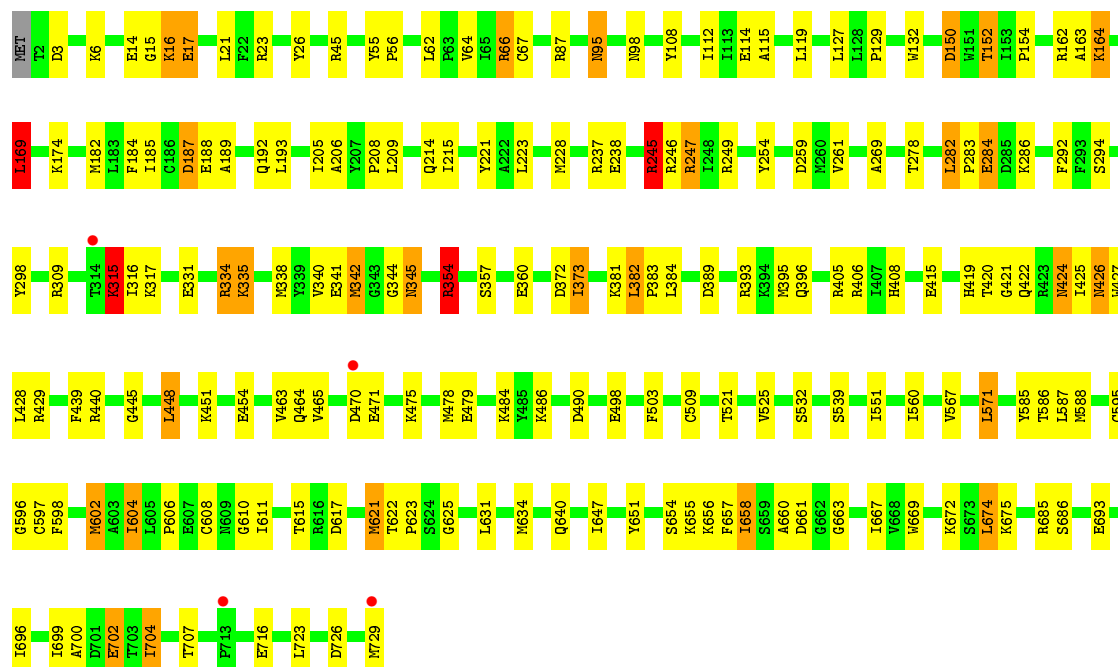


- Molecule 1: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit beta

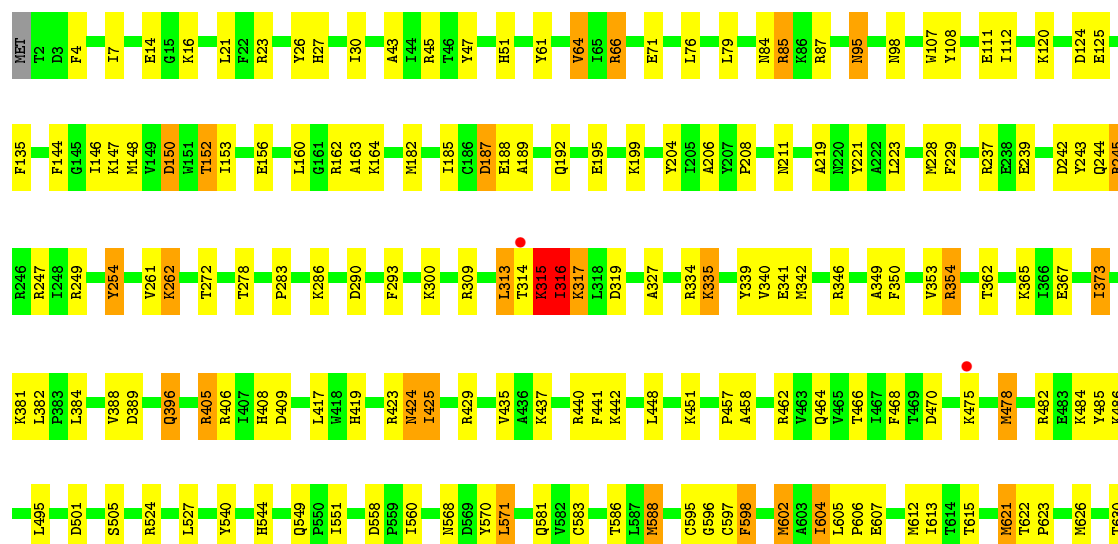




• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha

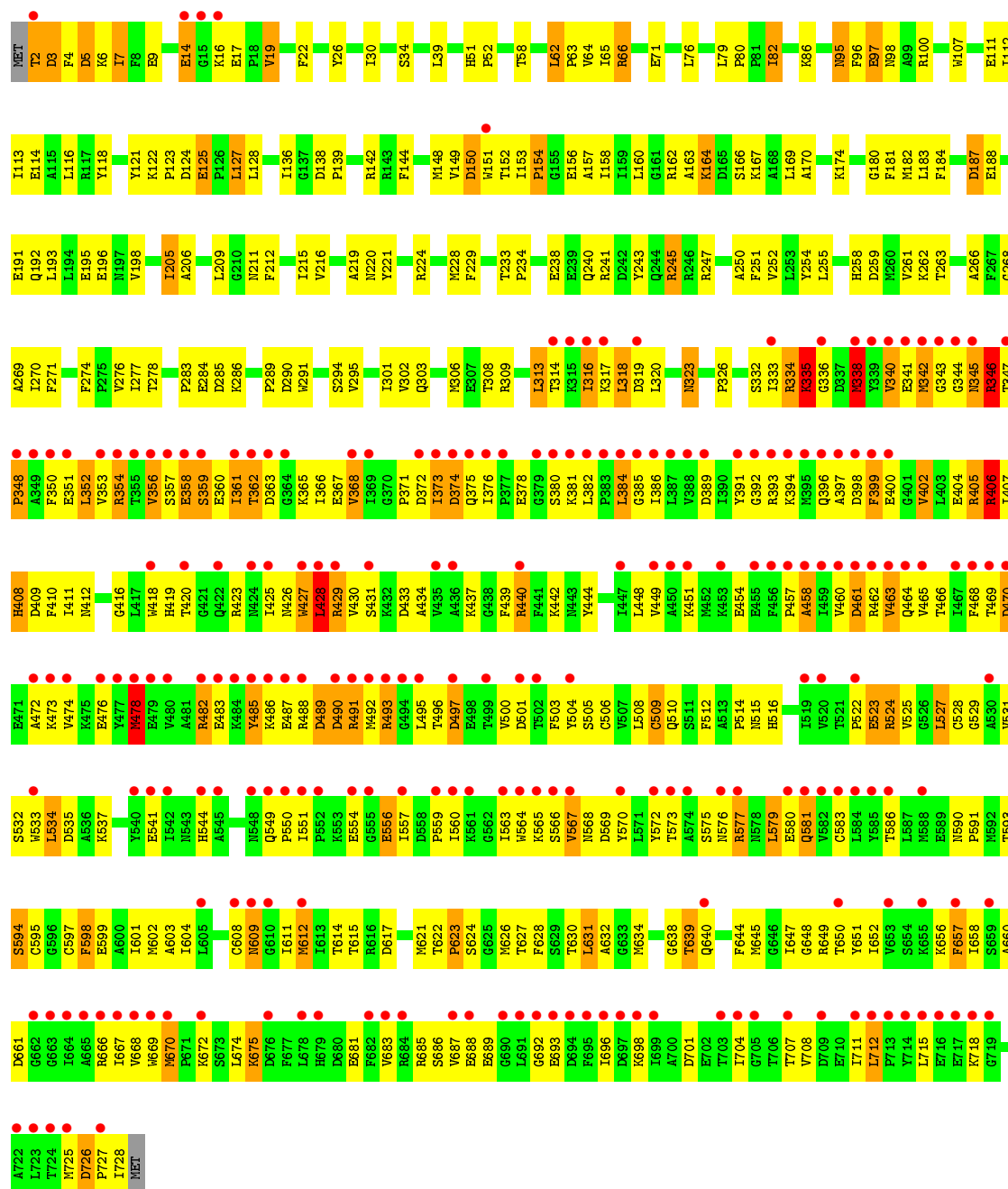
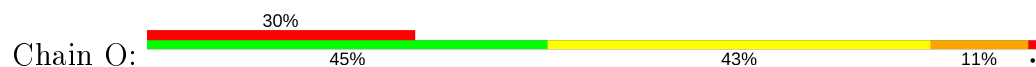


• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



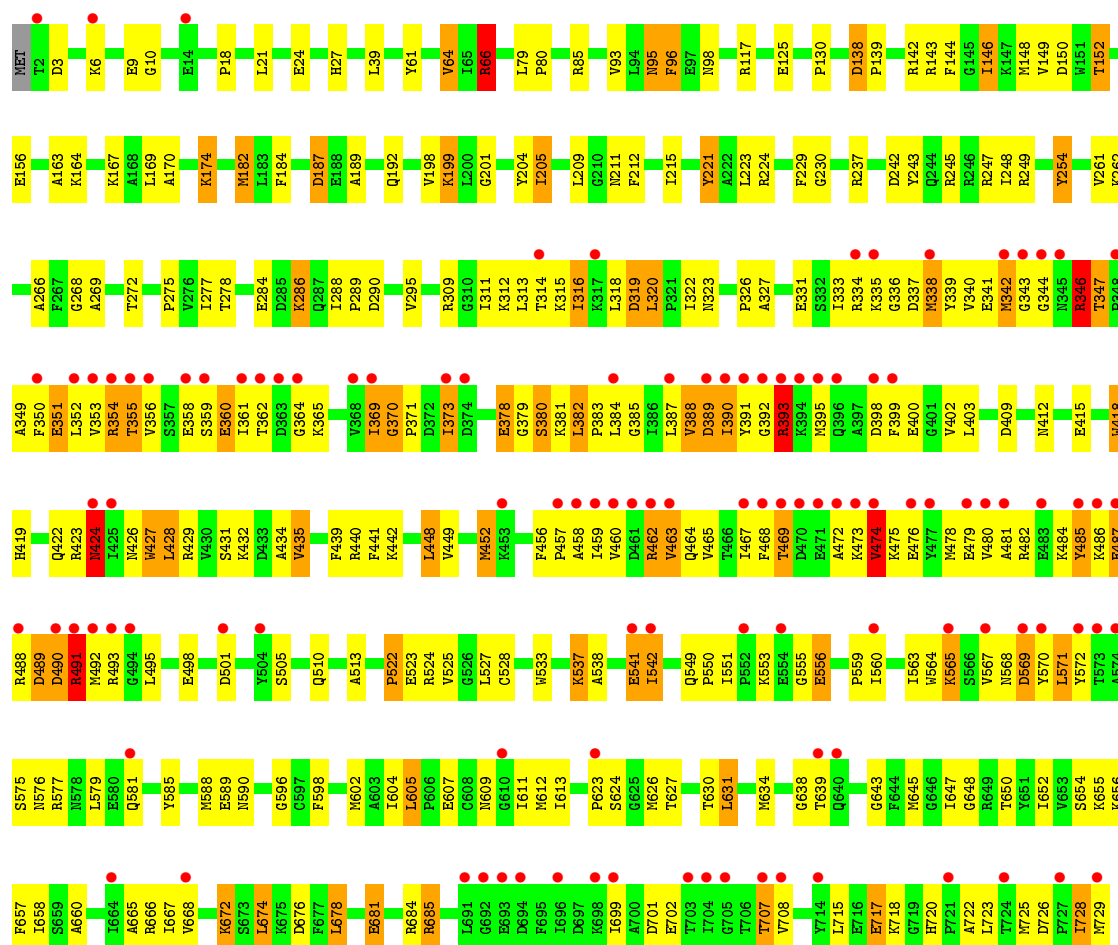


• Molecule 2: Carbon monoxide dehydrogenase/acetyl CoA synthase subunit alpha



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.54Å 136.60Å 141.75Å 101.29° 109.22° 103.91°	Depositor
Resolution (Å)	49.00 – 2.51 48.25 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.00-2.51) 95.0 (48.25-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 2.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.178 , 0.250 0.179 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	44706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: XCC, CU1, GOL, SF4, XE, NI

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.29	19/5187 (0.4%)	1.13	26/7028 (0.4%)
1	B	1.29	15/5187 (0.3%)	1.10	13/7028 (0.2%)
1	C	1.25	12/5187 (0.2%)	1.08	17/7028 (0.2%)
1	D	1.18	7/5187 (0.1%)	1.07	12/7028 (0.2%)
2	M	1.21	13/5874 (0.2%)	1.09	20/7954 (0.3%)
2	N	1.27	14/5874 (0.2%)	1.12	26/7954 (0.3%)
2	O	1.17	1/5859 (0.0%)	0.99	8/7937 (0.1%)
2	P	1.15	2/5874 (0.0%)	1.03	14/7954 (0.2%)
All	All	1.23	83/44229 (0.2%)	1.08	136/59911 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
2	N	0	1
2	P	0	1
All	All	0	7

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CG-CD	12.53	1.70	1.51
1	B	196	GLU	CG-CD	9.77	1.66	1.51
2	N	681	GLU	CG-CD	8.11	1.64	1.51
2	N	702	GLU	CB-CG	-7.98	1.36	1.52

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	114[A]	CYS	CB-SG	-7.91	1.68	1.82
2	N	681	GLU	CD-OE2	7.83	1.34	1.25
1	B	610	VAL	CB-CG2	7.78	1.69	1.52
1	A	126	GLU	CG-CD	7.52	1.63	1.51
2	M	188	GLU	CG-CD	7.47	1.63	1.51
2	N	693	GLU	CG-CD	7.39	1.63	1.51
1	A	628	TYR	CD1-CE1	-7.26	1.28	1.39
1	B	406	GLU	CG-CD	7.13	1.62	1.51
1	C	383	ALA	CA-CB	-7.08	1.37	1.52
1	C	664	GLU	CG-CD	7.02	1.62	1.51
1	A	102	VAL	CB-CG1	-6.97	1.38	1.52
2	N	120	LYS	CE-NZ	6.82	1.66	1.49
1	C	538	GLU	CG-CD	6.75	1.62	1.51
1	D	15	GLU	CG-CD	6.70	1.62	1.51
2	N	681	GLU	CD-OE1	6.67	1.32	1.25
2	M	597	CYS	CB-SG	-6.55	1.71	1.82
1	A	617	TYR	CD1-CE1	6.53	1.49	1.39
1	A	126	GLU	CD-OE1	6.44	1.32	1.25
1	B	500	CYS	CB-SG	6.31	1.93	1.82
1	A	397	ALA	CA-CB	-6.30	1.39	1.52
1	C	23	LYS	CD-CE	6.18	1.66	1.51
2	N	64	VAL	CB-CG2	-6.16	1.40	1.52
2	M	292	PHE	CE1-CZ	6.16	1.49	1.37
1	A	661	GLU	CG-CD	6.09	1.61	1.51
1	A	82	ASP	CB-CG	-6.06	1.39	1.51
1	D	137	VAL	CB-CG2	6.02	1.65	1.52
1	C	67	CYS	CB-SG	-6.00	1.72	1.82
2	M	284	GLU	CG-CD	6.00	1.60	1.51
1	D	353	VAL	CB-CG2	5.97	1.65	1.52
1	D	550	CYS	CB-SG	-5.90	1.72	1.81
2	N	239	GLU	CG-CD	5.90	1.60	1.51
2	M	269	ALA	CA-CB	5.86	1.64	1.52
1	A	538	GLU	CB-CG	5.82	1.63	1.52
2	M	26	TYR	CD1-CE1	-5.79	1.30	1.39
2	N	135	PHE	CE2-CZ	5.73	1.48	1.37
1	B	600	VAL	CB-CG1	-5.66	1.41	1.52
1	D	242	TYR	CD1-CE1	5.60	1.47	1.39
1	B	102	VAL	CB-CG1	-5.58	1.41	1.52
1	D	216	VAL	CB-CG2	-5.58	1.41	1.52
1	A	196	GLU	CG-CD	5.55	1.60	1.51
1	B	334	PHE	CE2-CZ	5.54	1.47	1.37
2	M	331[A]	GLU	CB-CG	-5.51	1.41	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	108	TYR	CE2-CZ	5.50	1.45	1.38
1	A	464	VAL	CB-CG2	-5.49	1.41	1.52
2	N	595	CYS	CB-SG	-5.48	1.72	1.81
2	N	524	ARG	CZ-NH2	5.47	1.40	1.33
1	B	664	GLU	CG-CD	5.41	1.60	1.51
1	C	145	GLU	CG-CD	5.41	1.60	1.51
1	B	196	GLU	CD-OE1	5.38	1.31	1.25
1	B	70	PHE	CE1-CZ	5.37	1.47	1.37
2	M	595	CYS	CB-SG	-5.36	1.73	1.81
1	A	383	ALA	CA-CB	-5.35	1.41	1.52
1	B	95	TRP	CG-CD1	-5.34	1.29	1.36
1	B	247	ILE	CB-CG2	5.34	1.69	1.52
2	M	509	CYS	CB-SG	-5.30	1.73	1.81
1	C	519	TYR	CG-CD1	5.30	1.46	1.39
1	C	406	GLU	CG-CD	5.27	1.59	1.51
2	M	14	GLU	CD-OE1	5.27	1.31	1.25
2	M	702	GLU	CB-CG	5.27	1.62	1.52
2	M	284	GLU	CB-CG	5.25	1.62	1.52
1	D	631	TYR	CB-CG	-5.24	1.43	1.51
2	P	418	TRP	CB-CG	5.22	1.59	1.50
2	M	187	ASP	CB-CG	5.22	1.62	1.51
1	C	520	CYS	CB-SG	-5.21	1.73	1.81
1	A	95	TRP	CE3-CZ3	5.21	1.47	1.38
1	A	159	VAL	CB-CG2	-5.19	1.42	1.52
2	N	293	PHE	CD2-CE2	5.16	1.49	1.39
2	N	71	GLU	CD-OE1	5.16	1.31	1.25
1	B	600	VAL	CB-CG2	-5.15	1.42	1.52
1	C	316	CYS	CB-SG	-5.13	1.73	1.81
1	C	23	LYS	CE-NZ	5.11	1.61	1.49
1	C	460	GLU	CD-OE1	5.09	1.31	1.25
2	P	93	VAL	CB-CG2	5.09	1.63	1.52
1	A	578	ALA	CA-CB	-5.09	1.41	1.52
2	O	97	GLU	CD-OE1	5.07	1.31	1.25
1	A	168	GLU	CB-CG	5.07	1.61	1.52
1	A	59	CYS	CB-SG	-5.03	1.73	1.81
1	B	522	ASP	CB-CG	5.03	1.62	1.51
1	A	168	GLU	CD-OE2	5.01	1.31	1.25

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	236	ARG	NE-CZ-NH2	-13.82	113.39	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	A	176	ARG	NE-CZ-NH1	10.58	125.59	120.30
2	N	237	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	N	621	MET	CG-SD-CE	-9.91	84.33	100.20
1	A	530	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	B	647	ASP	CB-CG-OD2	-9.15	110.06	118.30
1	A	176	ARG	NE-CZ-NH2	-9.13	115.74	120.30
2	O	241	ARG	NE-CZ-NH1	-8.96	115.82	120.30
2	N	409	ASP	CB-CG-OD2	8.88	126.29	118.30
1	A	647	ASP	CB-CG-OD1	-8.86	110.33	118.30
1	A	563	MET	CG-SD-CE	-8.82	86.08	100.20
2	P	85	ARG	NE-CZ-NH2	-8.48	116.06	120.30
2	M	237	ARG	NE-CZ-NH2	-8.21	116.19	120.30
2	M	162	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	D	339	LEU	CA-CB-CG	-8.17	96.52	115.30
2	M	162	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	M	45	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	N	237	ARG	NE-CZ-NH1	7.96	124.28	120.30
2	N	245	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	N	571	LEU	CA-CB-CG	7.86	133.38	115.30
2	P	242	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	B	236	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	352	ASP	CB-CG-OD1	7.54	125.09	118.30
2	M	23	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	236	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	194	ARG	NE-CZ-NH2	7.51	124.06	120.30
1	D	199	ARG	NE-CZ-NH1	7.45	124.03	120.30
2	P	249	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	C	236	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	D	148	ARG	NE-CZ-NH1	7.27	123.94	120.30
2	P	242	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	12	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	A	3	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	139	ASP	CB-CG-OD1	7.01	124.61	118.30
2	N	702	GLU	CB-CA-C	-6.96	96.47	110.40
1	A	331	VAL	CB-CA-C	-6.96	98.18	111.40
1	A	18	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	M	169	LEU	CB-CG-CD2	6.75	122.47	111.00
1	A	530	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	A	352	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	647	ASP	CB-CG-OD1	-6.67	112.29	118.30
2	N	597	CYS	CA-CB-SG	-6.67	102.00	114.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	66	ARG	NE-CZ-NH2	-6.66	116.97	120.30
2	M	354	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	331	VAL	CB-CA-C	-6.58	98.90	111.40
1	B	416	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	P	428	LEU	CA-CB-CG	6.50	130.25	115.30
1	D	87	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	25	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	D	236	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	376	ASP	CB-CG-OD1	6.38	124.04	118.30
2	N	524	ARG	NE-CZ-NH1	-6.37	117.11	120.30
2	N	406	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	D	82	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	D	647	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	A	77	ARG	NE-CZ-NH1	6.31	123.45	120.30
2	N	501	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	194	ARG	NE-CZ-NH1	-6.29	117.16	120.30
1	C	416	ARG	C-N-CD	6.23	141.48	128.40
2	N	85	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	P	224	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	N	150	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	149	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	176	ARG	NE-CZ-NH2	-6.16	117.22	120.30
2	P	247	ARG	NE-CZ-NH1	6.13	123.37	120.30
2	N	309	ARG	NE-CZ-NH2	6.12	123.36	120.30
2	M	249	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	500	CYS	CA-CB-SG	-6.11	103.00	114.00
2	P	66	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	458	ASP	CB-CG-OD1	6.03	123.72	118.30
2	N	85	ARG	CG-CD-NE	-5.97	99.26	111.80
2	O	346	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	236	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	N	631	LEU	CA-CB-CG	5.89	128.84	115.30
1	C	3	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	C	325	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	176	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	114[A]	CYS	CA-CB-SG	-5.81	103.55	114.00
2	M	247	ARG	NE-CZ-NH2	-5.81	117.40	120.30
2	M	484	LYS	CD-CE-NZ	-5.79	98.39	111.70
2	M	150	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	100	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	M	245	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	M	45	ARG	NE-CZ-NH1	5.68	123.14	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	249	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	O	661	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	P	85	ARG	CG-CD-NE	-5.63	99.97	111.80
2	P	66	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	51	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	387	ASP	CB-CG-OD2	5.62	123.35	118.30
1	D	149	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	475	GLY	N-CA-C	-5.59	99.12	113.10
2	M	282	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	C	250	ASP	CB-CG-OD1	5.53	123.28	118.30
2	M	490	ASP	CB-CG-OD1	5.51	123.26	118.30
2	P	138	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	349	MET	N-CA-C	-5.50	96.15	111.00
1	A	550	CYS	CA-CB-SG	-5.49	104.12	114.00
1	A	376	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	594	TRP	CA-CB-CG	5.44	124.03	113.70
2	N	346	ARG	NE-CZ-NH2	-5.43	117.59	120.30
2	N	409	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	149	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	C	221	MET	CG-SD-CE	5.41	108.86	100.20
2	N	602	MET	CG-SD-CE	-5.40	91.56	100.20
1	D	27	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	M	406	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	O	82	ILE	CG1-CB-CG2	-5.38	99.55	111.40
2	O	631	LEU	CA-CB-CG	5.34	127.58	115.30
2	N	319	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	471	ASN	N-CA-C	-5.31	96.66	111.00
2	N	245	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	12	ARG	NE-CZ-NH2	5.27	122.94	120.30
2	O	313	LEU	CA-CB-CG	5.27	127.41	115.30
1	D	199	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	77	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	C	274	ASP	CB-CG-OD1	5.22	123.00	118.30
2	M	597	CYS	CA-CB-SG	-5.22	104.59	114.00
1	D	352	ASP	CB-CG-OD1	5.21	122.98	118.30
2	N	242	ASP	CB-CG-OD2	5.20	122.98	118.30
2	N	680	ASP	CB-CG-OD1	5.20	122.98	118.30
2	O	338	MET	CA-CB-CG	5.17	122.10	113.30
2	P	452	MET	CG-SD-CE	5.17	108.48	100.20
2	M	119	LEU	CB-CG-CD2	5.17	119.79	111.00
1	B	550	CYS	CA-CB-SG	-5.17	104.70	114.00
2	O	661	ASP	CB-CG-OD1	5.13	122.92	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	ASP	CB-CG-OD1	5.13	122.92	118.30
2	P	167	LYS	CD-CE-NZ	5.12	123.48	111.70
1	C	426	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	P	237	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	M	334	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	N	697	ASP	CB-CG-OD1	5.05	122.85	118.30
2	N	23	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	522	ASP	CB-CG-OD1	5.02	122.82	118.30
1	C	355	CYS	CA-CB-SG	-5.02	104.96	114.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	SER	Peptide
1	B	469	GLY	Peptide
1	C	415	ASN	Peptide
1	C	469	GLY	Peptide
1	D	469	GLY	Peptide
2	N	313	LEU	Peptide
2	P	389	ASP	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5094	0	5088	114	0
1	B	5094	0	5082	133	0
1	C	5094	0	5086	140	0
1	D	5094	0	5093	154	0
2	M	5740	0	5693	116	0
2	N	5740	0	5695	127	0
2	O	5725	0	5680	308	0
2	P	5740	0	5693	243	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	5	0
3	P	8	0	0	1	0
4	A	9	0	0	2	0
4	B	9	0	0	3	0
4	C	9	0	0	3	0
4	D	9	0	0	1	0
5	A	7	0	0	11	0
5	B	7	0	0	12	0
5	C	7	0	0	7	0
5	D	7	0	0	6	0
5	M	3	0	0	2	0
5	N	4	0	0	5	0
5	O	3	0	0	4	0
5	P	4	0	0	4	0
6	A	24	0	32	4	0
6	B	18	0	24	5	0
6	C	12	0	16	1	0
6	D	12	0	16	7	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	1	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	A	168	0	0	5	0
9	B	220	0	0	12	0
9	C	130	0	0	14	0
9	D	105	0	0	11	0
9	M	201	0	0	9	0
9	N	222	0	0	20	0
9	O	27	0	0	5	0
9	P	80	0	0	8	0
All	All	44706	0	43198	1297	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 15.

All (1297) 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:114[A]:CYS:HB2	9:B:1217:HOH:O	1.29	1.28
2:O:373:ILE:HG22	2:O:440:ARG:HG3	1.28	1.09
1:B:148[A]:ARG:NH1	9:B:1185:HOH:O	1.78	1.08
1:D:114:CYS:HB2	9:D:1050:HOH:O	1.50	1.08
1:D:279:VAL:HG11	1:D:315:ILE:HD12	1.34	1.07
1:D:105:MET:CE	1:D:609:PRO:HD3	1.84	1.06
1:D:525:LYS:HE2	9:D:1094:HOH:O	1.57	1.04
1:A:577:VAL:HG21	1:A:645:ILE:HG23	1.41	0.98
2:O:144:PHE:O	2:O:148:MET:HG3	1.64	0.98
6:A:862:GOL:H31	2:M:259:ASP:HB3	1.44	0.97
2:O:698:LYS:HA	2:O:718:LYS:HG2	1.46	0.96
2:O:670:MET:HG2	2:O:674:LEU:HD23	1.48	0.95
1:C:587:LYS:H	1:D:220:HIS:HE1	1.13	0.95
2:N:722:ALA:HA	2:N:725:MET:HE3	1.49	0.95
2:P:354:ARG:HH21	2:P:356:VAL:CG1	1.80	0.94
2:P:384:LEU:HA	2:P:468:PHE:O	1.66	0.94
1:D:105:MET:HE2	1:D:609:PRO:CD	1.97	0.93
2:O:363:ASP:HB2	2:O:462:ARG:HD2	1.52	0.92
1:D:279:VAL:HG11	1:D:315:ILE:CD1	2.00	0.91
1:D:105:MET:HE2	1:D:609:PRO:HD3	1.50	0.90
1:B:577:VAL:HG21	1:B:645:ILE:HG23	1.53	0.90
1:B:110:ALA:O	1:B:114[A]:CYS:SG	2.30	0.89
2:O:334:ARG:HG3	9:O:1028:HOH:O	1.74	0.88
2:O:508:LEU:HB3	3:O:900:SF4:S1	2.14	0.88
1:B:400:ALA:HA	1:B:403:MET:HE3	1.57	0.87
1:C:620:LEU:HD23	5:C:1004:XE:XE	2.52	0.87
7:O:950:CU1:CU	5:O:1009:XE:XE	2.02	0.87
1:A:114:CYS:HB2	9:A:1134:HOH:O	1.73	0.86
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.39	0.86
2:O:407:ILE:HG23	2:O:408:HIS:H	1.40	0.86
1:D:335:ALA:H	1:D:471:ASN:HD22	1.19	0.85
2:N:163:ALA:H	2:N:192:GLN:HE22	1.25	0.85
1:C:114:CYS:HB2	9:C:1089:HOH:O	1.75	0.85
6:B:863:GOL:H32	2:N:27:HIS:CE1	2.12	0.85
1:C:126:GLU:OE1	1:C:390:THR:OG1	1.93	0.84
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.40	0.84
2:O:373:ILE:HG22	2:O:440:ARG:CG	2.08	0.84
1:B:400:ALA:HA	1:B:403:MET:CE	2.08	0.83
2:P:549:GLN:HG3	2:P:550:PRO:HD2	1.57	0.83
2:P:490:ASP:C	2:P:492:MET:H	1.80	0.83
2:M:696:ILE:HA	2:M:699:ILE:HD12	1.61	0.82
1:D:102:VAL:HG13	5:D:1003[B]:XE:XE	2.57	0.82

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:MET:CE	1:D:609:PRO:CD	2.56	0.81
2:P:522:PRO:HD3	2:P:533:TRP:CD1	2.15	0.81
1:B:114[A]:CYS:SG	9:B:1161:HOH:O	2.38	0.81
1:C:114:CYS:SG	1:C:209:HIS:CD2	2.73	0.81
2:O:371:PRO:HD2	2:O:469:THR:HB	1.63	0.79
2:O:468:PHE:HB2	2:O:474:VAL:HG23	1.63	0.79
1:C:620:LEU:HD21	5:C:1003[A]:XE:XE	2.61	0.79
1:D:470:CYS:HB3	4:D:800:XCC:S2	2.23	0.79
1:C:102:VAL:CG1	5:C:1003[B]:XE:XE	3.09	0.79
2:O:411:ILE:HD13	2:O:428:LEU:HD21	1.64	0.78
2:O:373:ILE:CG2	2:O:440:ARG:HG3	2.12	0.78
2:P:343:GLY:HA3	2:P:349:ALA:HB3	1.66	0.78
2:O:612:MET:SD	2:O:624:SER:HB3	2.24	0.78
1:C:411:ARG:HG3	1:C:416:ARG:HD3	1.64	0.78
2:P:95:ASN:C	2:P:95:ASN:HD22	1.86	0.78
2:M:451:LYS:NZ	2:M:454:GLU:OE1	2.14	0.77
2:O:396:GLN:HB2	2:O:399:PHE:CE2	2.18	0.77
1:C:114:CYS:SG	1:C:209:HIS:NE2	2.58	0.77
2:P:588:MET:CE	2:P:604:ILE:HD13	2.15	0.77
1:D:614:ASP:N	6:D:863:GOL:H11	2.00	0.77
2:M:163:ALA:H	2:M:192:GLN:HE22	1.33	0.76
1:C:563:MET:CE	1:C:576:PHE:HD2	1.97	0.76
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.50	0.76
2:O:6:LYS:HA	2:O:9:GLU:HG3	1.67	0.76
1:A:335:ALA:H	1:A:471:ASN:HD22	1.31	0.76
1:B:580:ALA:HB2	5:B:1001:XE:XE	2.62	0.76
1:A:294:ALA:O	1:A:298:MET:HG3	1.86	0.75
2:P:156:GLU:HG2	5:P:1008:XE:XE	2.64	0.75
1:A:622:GLN:HB3	6:A:862:GOL:H11	1.67	0.75
2:N:588:MET:HE2	2:N:728:ILE:HG12	1.69	0.75
2:M:640:GLN:HB2	9:M:1157:HOH:O	1.85	0.75
2:N:588:MET:HE1	2:N:604:ILE:HG23	1.69	0.75
2:P:525:VAL:HG11	2:P:650:THR:CG2	2.15	0.75
1:C:470:CYS:HB3	4:C:800:XCC:S2	2.27	0.75
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.22	0.75
2:O:407:ILE:CG2	2:O:408:HIS:H	1.98	0.74
2:O:14:GLU:HA	9:O:1027:HOH:O	1.86	0.74
2:O:333:ILE:HG21	2:O:429:ARG:HB3	1.69	0.74
2:P:555:GLY:HA3	2:P:565:LYS:HB3	1.69	0.74
2:O:406:ARG:O	2:O:410:PHE:CD2	2.41	0.74
1:A:577:VAL:HG21	1:A:645:ILE:CG2	2.18	0.74

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.69	0.74
1:D:302:ALA:O	1:D:307:ALA:HB3	1.89	0.73
1:D:279:VAL:CG1	1:D:315:ILE:HD12	2.16	0.73
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.22	0.73
2:N:621:MET:HE1	9:N:1020:HOH:O	1.87	0.73
2:P:381:LYS:O	2:P:382:LEU:HD13	1.87	0.73
1:D:525:LYS:CE	9:D:1094:HOH:O	2.25	0.73
2:P:568:ASN:HD21	2:P:581:GLN:HG3	1.52	0.73
1:A:68:CYS:HB2	1:A:97:ILE:HG23	1.71	0.73
1:C:563:MET:HE2	1:C:576:PHE:HD2	1.53	0.72
1:A:33:VAL:HG21	1:A:477:GLN:HE22	1.54	0.72
2:M:344:GLY:O	2:M:345:ASN:HB2	1.88	0.72
1:C:2:PRO:N	1:C:625:SER:HG	1.86	0.72
2:O:469:THR:O	2:O:470:ASP:HB2	1.88	0.72
1:C:51:ARG:HD3	9:C:1137:HOH:O	1.89	0.72
2:O:418:TRP:O	2:O:428:LEU:HA	1.90	0.72
2:P:163:ALA:H	2:P:192:GLN:HE22	1.38	0.72
2:M:189:ALA:HA	2:M:192:GLN:HE21	1.53	0.72
1:D:32:ALA:HB1	1:D:268:MET:HG3	1.72	0.72
2:N:229:PHE:CD1	5:N:1009:XE:XE	3.21	0.71
2:O:407:ILE:HG23	2:O:408:HIS:N	2.05	0.71
2:P:95:ASN:ND2	2:P:98:ASN:H	1.87	0.71
1:D:114:CYS:SG	1:D:209:HIS:CD2	2.83	0.71
2:P:354:ARG:HH21	2:P:356:VAL:HG13	1.54	0.71
1:D:614:ASP:H	6:D:863:GOL:H11	1.55	0.71
1:C:102:VAL:HG13	5:C:1003[B]:XE:XE	2.69	0.71
1:C:105:MET:HE1	1:C:609:PRO:HD3	1.71	0.71
2:O:361:ILE:HD13	2:O:391:TYR:HB2	1.73	0.71
2:P:383:PRO:HB2	2:P:474:VAL:HG21	1.73	0.71
2:P:560:ILE:O	2:P:660:ALA:HB2	1.90	0.71
1:B:77:ARG:HD3	9:B:1199:HOH:O	1.90	0.71
1:A:105:MET:HE1	1:B:72:MET:CG	2.21	0.71
1:C:620:LEU:CD2	5:C:1004:XE:XE	3.17	0.70
2:M:408:HIS:HD2	2:M:419:HIS:ND1	1.90	0.70
2:O:524:ARG:NH2	2:O:645:MET:HE1	2.07	0.70
2:P:568:ASN:ND2	2:P:581:GLN:HA	2.07	0.70
2:N:150:ASP:OD1	2:N:152:THR:HG23	1.92	0.70
2:N:588:MET:CE	2:N:728:ILE:HG12	2.21	0.70
2:O:341:GLU:OE2	2:O:343:GLY:N	2.22	0.70
2:O:346:ARG:HH11	2:O:346:ARG:HB2	1.56	0.70
2:O:429:ARG:N	9:O:1018:HOH:O	2.25	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:364:ALA:HB1	1:D:369:THR:HB	1.74	0.70
2:O:580:GLU:O	2:O:581:GLN:HB2	1.90	0.70
2:O:62:LEU:HD12	2:O:65:ILE:HD12	1.72	0.70
1:C:577:VAL:HG21	1:C:645:ILE:HG23	1.73	0.69
2:M:150:ASP:OD1	2:M:152:THR:HG23	1.92	0.69
1:C:416:ARG:HD2	1:C:418:VAL:HG23	1.74	0.69
2:P:150:ASP:OD1	2:P:152:THR:HG23	1.92	0.69
1:A:2:PRO:N	6:A:862:GOL:HO1	1.89	0.69
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.26	0.69
1:D:102:VAL:CG1	5:D:1003[B]:XE:XE	3.19	0.69
1:D:65:GLY:HA2	9:D:1089:HOH:O	1.92	0.69
2:N:261:VAL:HG12	5:N:1006:XE:XE	2.70	0.69
1:A:24:ASN:O	1:A:27:ARG:HG2	1.93	0.69
1:B:470:CYS:HB3	4:B:800:XCC:S2	2.32	0.69
2:O:252:VAL:HB	2:O:276:VAL:HG22	1.74	0.69
2:O:509:CYS:SG	2:O:595:CYS:SG	2.91	0.69
1:C:482:LEU:HD13	1:C:486:LYS:HD2	1.75	0.69
1:B:577:VAL:HG21	1:B:645:ILE:CG2	2.23	0.68
1:B:416:ARG:HG3	1:B:416:ARG:HH11	1.56	0.68
1:C:78:ILE:HD11	1:C:97:ILE:HD12	1.75	0.68
2:M:415:GLU:OE1	9:M:1206:HOH:O	2.11	0.68
2:O:491:ARG:HH11	2:O:491:ARG:HB2	1.58	0.68
2:O:675:LYS:HA	2:O:696:ILE:HD11	1.75	0.68
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.75	0.68
2:M:3:ASP:CG	9:M:1198:HOH:O	2.32	0.68
2:M:445:GLY:HA2	2:M:465:VAL:HG11	1.76	0.67
1:C:12:ARG:O	6:C:861:GOL:H12	1.94	0.67
2:O:649:ARG:O	2:O:652:ILE:HD12	1.94	0.67
2:O:96:PHE:O	2:O:100:ARG:HG3	1.95	0.67
2:P:474:VAL:CG1	2:P:475:LYS:N	2.58	0.67
1:B:510:LEU:N	1:B:510:LEU:HD12	2.08	0.67
2:M:373:ILE:CG2	2:M:440:ARG:HD3	2.25	0.66
2:P:338:MET:SD	2:P:341:GLU:HB2	2.35	0.66
1:A:280:LEU:HD13	1:A:288:SER:HB2	1.77	0.66
1:B:468:CYS:SG	5:B:1001:XE:XE	3.32	0.66
2:N:354:ARG:HD2	2:N:389:ASP:OD1	1.95	0.66
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.78	0.66
2:P:143:ARG:O	2:P:146[A]:ILE:HD13	1.95	0.66
1:A:105:MET:CE	1:B:72:MET:HG3	2.25	0.66
1:C:159:VAL:HG13	9:C:1052:HOH:O	1.95	0.66
2:O:516:HIS:CD2	2:O:593:THR:OG1	2.49	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.10	0.66
1:D:470:CYS:O	1:D:582:GLU:HB2	1.94	0.66
2:O:316:ILE:HG23	2:O:316:ILE:O	1.96	0.66
2:O:649:ARG:HA	2:O:652:ILE:CD1	2.26	0.66
2:N:315:LYS:HD3	9:N:1162:HOH:O	1.95	0.65
2:P:474:VAL:CG1	2:P:475:LYS:H	2.10	0.65
2:P:316:ILE:HG23	2:P:316:ILE:O	1.96	0.65
1:A:105:MET:HE1	1:B:72:MET:HG3	1.78	0.65
1:B:400:ALA:HB2	5:B:1010:XE:XE	2.75	0.65
1:C:442:THR:HG21	1:C:537:ILE:HD11	1.79	0.65
2:M:428:LEU:N	2:M:428:LEU:HD12	2.11	0.65
2:P:387:LEU:O	2:P:465:VAL:HA	1.96	0.65
1:C:587:LYS:H	1:D:220:HIS:CE1	2.05	0.65
2:O:556:GLU:HG2	2:O:557:ILE:N	2.12	0.65
1:D:105:MET:HE2	1:D:609:PRO:CG	2.26	0.65
2:M:617:ASP:HB2	9:M:1199:HOH:O	1.97	0.65
2:M:15:GLY:O	2:M:16:LYS:HD3	1.97	0.65
2:N:722:ALA:HA	2:N:725:MET:CE	2.26	0.65
2:O:374:ASP:HB2	2:O:440:ARG:HE	1.62	0.65
2:P:189:ALA:HA	2:P:192:GLN:HE21	1.62	0.65
1:A:102:VAL:CG1	5:A:1003[B]:XE:XE	3.24	0.64
1:A:220:HIS:HE1	1:B:587:LYS:H	1.43	0.64
2:N:146:ILE:HG13	2:N:146:ILE:O	1.96	0.64
2:P:490:ASP:C	2:P:492:MET:N	2.50	0.64
2:O:568:ASN:ND2	2:O:581:GLN:HG2	2.12	0.64
2:O:346:ARG:NH1	2:O:346:ARG:HB2	2.12	0.64
2:P:489:ASP:HA	2:P:492:MET:HB2	1.79	0.64
1:B:287:LEU:CD1	1:B:388:TYR:CE1	2.81	0.64
1:C:640:VAL:HG12	1:C:644:LYS:HE3	1.80	0.64
2:O:351:GLU:HA	2:O:386:ILE:HB	1.79	0.64
1:B:316:CYS:H	1:B:503:GLN:HE22	1.45	0.64
2:O:556:GLU:HG2	2:O:557:ILE:H	1.63	0.64
2:O:580:GLU:O	2:O:581:GLN:CB	2.46	0.64
2:O:334:ARG:HH11	2:O:335:LYS:HG3	1.63	0.63
2:O:2:THR:HA	2:O:5:ASP:HB2	1.81	0.63
1:D:500:CYS:HA	1:D:503:GLN:HG3	1.79	0.63
2:P:666:ARG:HD2	2:P:728:ILE:HD13	1.80	0.63
1:A:357:MET:HG2	1:B:90:CYS:O	1.98	0.63
1:C:335:ALA:H	1:C:471:ASN:HD22	1.45	0.63
1:D:416:ARG:HB2	1:D:418:VAL:HG23	1.80	0.63
2:M:95:ASN:ND2	2:M:98:ASN:H	1.95	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.29	0.63
2:P:522:PRO:HD3	2:P:533:TRP:CG	2.34	0.63
2:P:95:ASN:HD21	2:P:98:ASN:H	1.46	0.63
1:A:15:GLU:OE2	6:A:861:GOL:H12	1.99	0.63
2:P:474:VAL:HG13	2:P:475:LYS:N	2.14	0.62
1:C:316:CYS:H	1:C:503:GLN:HE22	1.47	0.62
1:C:615:LEU:HD23	1:C:615:LEU:O	1.99	0.62
1:D:658:VAL:O	1:D:662:VAL:HG23	1.99	0.62
2:M:498:GLU:OE2	2:M:656:LYS:NZ	2.27	0.62
2:O:556:GLU:HA	2:O:564:TRP:CD1	2.35	0.62
2:N:396:GLN:NE2	9:N:1215:HOH:O	2.30	0.62
2:O:384:LEU:HD12	2:O:385:GLY:H	1.65	0.62
6:B:863:GOL:H32	2:N:27:HIS:HE1	1.62	0.62
2:O:556:GLU:HA	2:O:564:TRP:HD1	1.63	0.62
1:B:281:HIS:HB3	1:B:351:VAL:HG12	1.82	0.62
2:O:333:ILE:HG21	2:O:429:ARG:CB	2.30	0.62
2:O:149:VAL:HG11	2:O:509:CYS:HA	1.81	0.62
2:P:605:LEU:HD21	2:P:623:PRO:HB2	1.80	0.62
1:B:335:ALA:H	1:B:471:ASN:HD22	1.46	0.62
2:O:346:ARG:HG3	2:O:381:LYS:NZ	2.15	0.62
2:M:621:MET:HE1	2:M:622:THR:O	1.99	0.61
1:C:11:CYS:HB2	1:C:621:THR:HB	1.83	0.61
1:D:182:GLU:HG2	1:D:204:VAL:HG11	1.82	0.61
2:O:488:ARG:C	2:O:490:ASP:H	2.02	0.61
1:C:12:ARG:HD3	9:C:1107:HOH:O	1.99	0.61
2:N:373:ILE:HD12	2:N:441:PHE:CZ	2.35	0.61
2:O:221:TYR:CA	2:O:224:ARG:HH21	2.13	0.61
2:O:431:SER:O	2:O:434:ALA:N	2.24	0.61
1:A:7:LEU:HD11	2:M:164:LYS:HB2	1.83	0.61
2:P:187:ASP:HA	2:P:211:ASN:ND2	2.15	0.61
2:N:156:GLU:HG3	2:N:182:MET:HB3	1.82	0.61
2:O:221:TYR:HA	2:O:224:ARG:HH21	1.66	0.61
2:P:174:LYS:HE2	2:P:323:ASN:OD1	2.00	0.61
1:B:102:VAL:HG13	5:B:1003[B]:XE:XE	2.79	0.61
1:D:272:ASP:OD2	1:D:275:GLN:NE2	2.33	0.61
2:O:468:PHE:CB	2:O:474:VAL:HG23	2.31	0.61
2:P:164:LYS:NZ	9:P:1089:HOH:O	2.34	0.61
2:N:728:ILE:O	2:N:729:MET:HB2	1.98	0.61
2:P:611:ILE:HG13	2:P:611:ILE:O	2.01	0.61
2:N:300:LYS:HD2	9:N:1202:HOH:O	2.01	0.60
2:O:698:LYS:HA	2:O:718:LYS:CG	2.27	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HG	1:A:563:MET:CE	2.31	0.60
2:P:681:GLU:HG3	2:P:684:ARG:HH21	1.64	0.60
1:B:220:HIS:HD2	1:B:221:MET:O	1.85	0.60
1:C:273:PRO:HD3	1:C:420:ILE:HD12	1.83	0.60
2:M:585:TYR:CZ	2:M:656:LYS:HE3	2.36	0.60
2:P:354:ARG:NH2	2:P:356:VAL:CG1	2.59	0.60
1:B:287:LEU:HD13	1:B:388:TYR:CE1	2.37	0.60
2:O:334:ARG:HH11	2:O:335:LYS:CG	2.14	0.60
2:O:549:GLN:HB3	2:O:550:PRO:HD2	1.83	0.60
2:O:560:ILE:O	2:O:660:ALA:HB2	2.01	0.60
2:P:342:MET:CG	2:P:384:LEU:HD22	2.31	0.60
1:B:114[A]:CYS:CB	9:B:1161:HOH:O	2.50	0.60
2:P:672:LYS:HE3	2:P:676:ASP:OD2	2.01	0.60
2:M:587:LEU:HD23	2:M:588:MET:CE	2.32	0.60
1:C:7:LEU:HD11	2:O:164:LYS:HB2	1.84	0.60
1:A:2:PRO:N	1:A:625:SER:HG	2.00	0.60
1:A:602:THR:CG2	5:A:1001:XE:XE	3.28	0.60
1:B:114[A]:CYS:HB3	9:B:1161:HOH:O	2.01	0.60
1:B:325:ARG:HD2	9:B:1067:HOH:O	2.02	0.60
2:N:124:ASP:OD2	2:N:125:GLU:HB2	2.02	0.60
2:N:163:ALA:N	2:N:192:GLN:HE22	1.96	0.60
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.67	0.59
2:O:602:MET:HE1	2:O:647:ILE:HG21	1.83	0.59
2:P:523:GLU:O	2:P:654:SER:OG	2.17	0.59
1:A:102:VAL:HG13	5:A:1003[B]:XE:XE	2.80	0.59
1:D:114:CYS:SG	1:D:209:HIS:NE2	2.74	0.59
1:D:281:HIS:HB3	1:D:351:VAL:HG12	1.84	0.59
2:M:424:ASN:H	2:M:424:ASN:HD22	1.48	0.59
2:P:391:TYR:HD2	2:P:462:ARG:NH1	2.00	0.59
2:P:588:MET:HE1	2:P:604:ILE:HD13	1.84	0.59
1:C:294:ALA:O	1:C:298:MET:HG2	2.00	0.59
2:O:221:TYR:HA	2:O:224:ARG:NH2	2.18	0.59
2:O:429:ARG:HG3	9:O:1018:HOH:O	2.02	0.59
2:P:389:ASP:O	2:P:463:VAL:HA	2.01	0.59
2:P:525:VAL:HG11	2:P:650:THR:HG23	1.83	0.59
2:O:407:ILE:CG2	2:O:408:HIS:N	2.65	0.59
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.37	0.59
1:C:114:CYS:CB	9:C:1089:HOH:O	2.43	0.59
1:C:384:TYR:H	1:C:384:TYR:HD1	1.51	0.59
2:N:718:LYS:HD2	9:N:1200:HOH:O	2.03	0.59
1:B:298:MET:HE1	1:B:301:GLU:OE2	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:602:MET:CE	2:M:647:ILE:HG21	2.33	0.59
2:O:170:ALA:O	2:O:174:LYS:HB2	2.02	0.59
2:P:720:HIS:O	2:P:723:LEU:HB2	2.03	0.59
1:B:641:ALA:O	1:B:645:ILE:HG13	2.02	0.58
2:M:587:LEU:HD23	2:M:588:MET:HE2	1.85	0.58
2:O:250:ALA:H	2:O:309:ARG:HE	1.50	0.58
2:O:346:ARG:HG3	2:O:381:LYS:HZ1	1.68	0.58
2:O:698:LYS:CA	2:O:718:LYS:HG2	2.29	0.58
2:P:484:LYS:HA	2:P:487:GLU:HG3	1.84	0.58
2:P:565:LYS:HD2	2:P:569:ASP:OD1	2.03	0.58
1:D:472:ASN:O	1:D:474:LYS:N	2.36	0.58
2:N:457:PRO:O	2:N:458:ALA:HB3	2.03	0.58
2:O:516:HIS:HD2	2:O:593:THR:OG1	1.85	0.58
2:P:602:MET:HE1	2:P:645:MET:HE3	1.85	0.58
1:D:235:ILE:HG23	1:D:597:SER:OG	2.03	0.58
2:P:344:GLY:O	2:P:346:ARG:NH2	2.36	0.58
2:P:537:LYS:HD3	2:P:541:GLU:OE2	2.03	0.58
2:P:95:ASN:C	2:P:95:ASN:ND2	2.56	0.58
1:B:102:VAL:CG1	5:B:1003[B]:XE:XE	3.29	0.58
1:C:280:LEU:HD13	1:C:288:SER:HB2	1.86	0.58
2:M:338:MET:SD	2:M:341:GLU:HB2	2.44	0.58
2:M:372:ASP:OD1	2:M:373:ILE:N	2.32	0.58
2:M:342:MET:HG3	2:M:384:LEU:HD22	1.86	0.58
2:M:354:ARG:HD2	2:M:389:ASP:OD1	2.04	0.58
2:N:261:VAL:CG1	5:N:1006:XE:XE	3.30	0.58
2:O:508:LEU:HD23	3:O:900:SF4:S1	2.43	0.58
2:P:144:PHE:O	2:P:148:MET:HG3	2.02	0.58
2:P:602:MET:HE1	2:P:645:MET:CE	2.33	0.58
1:A:278:PHE:HB3	1:A:312:LEU:HD23	1.84	0.58
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.38	0.58
2:M:315:LYS:HB2	9:M:1182:HOH:O	2.02	0.58
2:O:506:CYS:SG	2:O:508:LEU:HB2	2.42	0.58
2:O:525:VAL:HG13	2:O:531:VAL:O	2.04	0.58
2:P:602:MET:CE	2:P:645:MET:HB3	2.34	0.58
2:M:357:SER:OG	2:M:360:GLU:HG2	2.04	0.58
2:O:433:ASP:O	2:O:437:LYS:HG3	2.04	0.58
2:P:295:VAL:HG12	2:P:295:VAL:O	2.03	0.58
2:P:391:TYR:HA	2:P:395:MET:HG2	1.83	0.58
2:O:405:ARG:HH22	2:O:532:SER:HB3	1.67	0.58
1:C:573:LYS:HE2	1:C:671:CYS:O	2.04	0.57
6:D:863:GOL:H12	2:P:27:HIS:CE1	2.39	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:156:GLU:HG3	2:O:182:MET:HB3	1.85	0.57
2:O:524:ARG:HH22	2:O:645:MET:HE1	1.69	0.57
1:D:525:LYS:NZ	9:D:1094:HOH:O	2.33	0.57
2:M:164:LYS:HD2	2:M:298:TYR:CE1	2.39	0.57
2:N:602:MET:HE2	2:N:647:ILE:HD13	1.85	0.57
2:P:369:ILE:HG22	2:P:370:GLY:H	1.69	0.57
1:A:114:CYS:SG	1:A:209:HIS:NE2	2.77	0.57
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.34	0.57
2:O:3:ASP:O	2:O:6:LYS:HG2	2.04	0.57
2:O:461:ASP:O	2:O:462:ARG:HG2	2.04	0.57
2:P:391:TYR:HD2	2:P:462:ARG:HH12	1.51	0.57
2:M:716:GLU:HG3	2:M:723:LEU:CD1	2.35	0.57
1:B:19:VAL:HG22	1:B:474:LYS:HG2	1.87	0.57
2:O:396:GLN:H	2:O:399:PHE:HD2	1.51	0.57
2:O:623:PRO:HB3	2:O:707:THR:C	2.25	0.57
2:P:479:GLU:O	2:P:481:ALA:N	2.37	0.57
1:D:530:ARG:HG3	1:D:530:ARG:HH11	1.69	0.57
1:D:105:MET:HE2	1:D:609:PRO:HG3	1.86	0.57
2:N:45:ARG:HD2	9:N:1216:HOH:O	2.03	0.57
2:O:316:ILE:HG22	2:O:454:GLU:OE1	2.04	0.57
1:D:98:VAL:HG21	1:D:613:SER:HB3	1.87	0.57
1:D:577:VAL:HG21	1:D:645:ILE:HG23	1.86	0.56
2:P:459:ILE:HG22	2:P:460:VAL:HG23	1.87	0.56
1:A:602:THR:HG23	5:A:1001:XE:XE	2.83	0.56
2:O:389:ASP:HB2	2:O:464:GLN:HB3	1.87	0.56
2:P:352:LEU:CD1	2:P:353:VAL:O	2.54	0.56
1:A:114:CYS:SG	1:A:209:HIS:CD2	2.98	0.56
1:D:36:MET:HE1	1:D:343:THR:HA	1.87	0.56
2:M:261:VAL:HG12	5:M:1006:XE:XE	2.83	0.56
2:N:21:LEU:HB2	2:N:286:LYS:HA	1.87	0.56
2:P:369:ILE:CG2	2:P:370:GLY:N	2.68	0.56
1:C:126:GLU:HG3	1:C:131:LYS:HB2	1.87	0.56
2:P:352:LEU:HD11	2:P:353:VAL:O	2.05	0.56
2:P:626:MET:HB3	2:P:630:THR:HB	1.88	0.56
1:A:313:VAL:HB	1:A:331:VAL:HG22	1.88	0.56
1:B:15:GLU:HA	6:B:861:GOL:H12	1.88	0.56
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.38	0.56
1:D:357:MET:O	1:D:360:ILE:HG12	2.05	0.56
2:M:420:THR:HG22	2:M:427:TRP:HB3	1.88	0.56
1:C:30:ASP:OD2	1:C:507:LYS:NZ	2.30	0.56
2:O:352:LEU:HD23	2:O:353:VAL:O	2.06	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:408:HIS:HA	2:O:419:HIS:ND1	2.21	0.56
2:O:510:GLN:O	2:O:514:PRO:HA	2.04	0.56
2:O:594:SER:HB3	2:O:598:PHE:HD2	1.70	0.56
2:P:318:LEU:HD22	2:P:320:LEU:HG	1.86	0.56
1:A:213:SER:OG	1:B:209:HIS:HD2	1.89	0.56
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.70	0.56
1:D:303:LYS:HA	1:D:307:ALA:O	2.06	0.56
2:O:359:SER:O	2:O:360:GLU:HB2	2.06	0.56
2:O:376:ILE:HG12	2:O:382:LEU:HD21	1.86	0.56
2:O:449:VAL:HG12	2:O:449:VAL:O	2.05	0.56
1:C:563:MET:HE2	1:C:576:PHE:CD2	2.38	0.56
2:M:657:PHE:O	2:M:658:ILE:C	2.44	0.56
2:O:180:GLY:HA2	2:O:326:PRO:HG2	1.88	0.56
2:P:347:THR:OG1	2:P:383:PRO:HA	2.06	0.56
1:B:235:ILE:HD11	5:B:1004:XE:XE	2.84	0.56
1:B:190:ILE:HG13	1:B:195:LYS:HG3	1.86	0.56
1:B:334:PHE:O	1:B:337:GLN:HG2	2.06	0.56
2:O:66:ARG:HG3	2:O:234:PRO:HB3	1.86	0.56
2:P:474:VAL:HG12	2:P:475:LYS:H	1.71	0.56
1:D:220:HIS:HD2	1:D:221:MET:O	1.89	0.56
2:M:357:SER:OG	2:M:360:GLU:CG	2.54	0.56
2:O:478:MET:HG3	2:O:482:ARG:HH21	1.71	0.56
2:M:17:GLU:HG2	9:M:1179:HOH:O	2.05	0.56
2:O:564:TRP:HB2	2:O:567:VAL:HB	1.88	0.56
2:N:588:MET:HE2	2:N:728:ILE:CG1	2.37	0.55
2:P:390:ILE:CG1	2:P:460:VAL:HG13	2.36	0.55
1:B:298:MET:CE	1:B:301:GLU:OE2	2.54	0.55
2:N:373:ILE:HG12	2:N:435:VAL:HG22	1.88	0.55
2:N:486:LYS:HG2	9:N:1156:HOH:O	2.05	0.55
2:O:515:ASN:OD1	2:O:576:ASN:HB2	2.06	0.55
2:O:522:PRO:HD3	2:O:533:TRP:CD1	2.41	0.55
2:P:343:GLY:HA2	2:P:347:THR:O	2.06	0.55
2:P:605:LEU:HD22	2:P:612:MET:HG2	1.88	0.55
1:C:209:HIS:HD2	1:D:213:SER:OG	1.89	0.55
2:M:108:TYR:O	2:M:112:ILE:HG13	2.06	0.55
2:N:341:GLU:HG3	2:N:429:ARG:HG2	1.89	0.55
2:P:369:ILE:CG2	2:P:370:GLY:H	2.20	0.55
1:A:620:LEU:CD2	5:A:1004:XE:XE	3.33	0.55
2:N:150:ASP:OD1	2:N:152:THR:CG2	2.55	0.55
2:O:254:TYR:CZ	2:O:258:HIS:CD2	2.94	0.55
2:P:390:ILE:HG13	2:P:460:VAL:HG13	1.89	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:484:LYS:HA	2:P:487:GLU:CG	2.36	0.55
1:B:480:SER:HA	1:B:638:PRO:HB3	1.88	0.55
2:N:505:SER:HB3	2:N:551:ILE:HD11	1.87	0.55
2:O:472:ALA:O	2:O:476:GLU:HB2	2.07	0.55
1:B:283:HIS:NE2	1:B:587:LYS:NZ	2.55	0.55
2:O:418:TRP:HZ3	2:O:429:ARG:NE	2.05	0.55
1:C:281:HIS:HB3	1:C:351:VAL:HG12	1.89	0.55
2:P:254:TYR:O	2:P:278:THR:HA	2.07	0.55
2:P:373:ILE:HG13	2:P:441:PHE:CZ	2.42	0.55
1:A:142:LYS:HD3	1:A:253:ASP:HB3	1.89	0.55
1:A:368:HIS:HB2	9:A:1141:HOH:O	2.06	0.55
2:N:95:ASN:ND2	2:N:98:ASN:H	2.05	0.55
2:O:670:MET:O	2:O:701:ASP:HB3	2.07	0.55
1:A:615:LEU:C	1:A:615:LEU:HD23	2.27	0.54
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.22	0.54
1:D:470:CYS:N	9:D:1085:HOH:O	2.39	0.54
2:N:602:MET:HE3	2:N:647:ILE:HG21	1.89	0.54
1:B:394:ILE:O	1:B:398:LYS:HG3	2.07	0.54
1:C:122:HIS:HD2	9:C:1127:HOH:O	1.88	0.54
2:M:615:THR:HG21	2:M:674:LEU:HG	1.89	0.54
2:P:21:LEU:HB2	2:P:286:LYS:HA	1.89	0.54
2:O:525:VAL:HG22	2:O:532:SER:HA	1.90	0.54
2:O:51:HIS:HB3	2:O:76:LEU:HD12	1.89	0.54
2:P:338:MET:CE	2:P:341:GLU:HB2	2.37	0.54
1:D:620:LEU:HD21	5:D:1003[A]:XE:XE	2.85	0.54
2:N:568:ASN:HD21	2:N:581:GLN:HE21	1.55	0.54
2:N:605:LEU:HD11	2:N:612:MET:HB3	1.89	0.54
1:D:208:ILE:HG21	9:D:1050:HOH:O	2.07	0.54
1:C:587:LYS:N	1:D:220:HIS:HE1	1.94	0.54
1:D:267:ASN:N	1:D:330:LEU:O	2.41	0.54
2:O:593:THR:HB	2:O:638:GLY:HA2	1.89	0.54
1:A:72:MET:HG3	1:B:105:MET:CE	2.37	0.54
2:O:113:ILE:O	2:O:116:LEU:HB2	2.07	0.54
1:D:281:HIS:O	1:D:351:VAL:HA	2.07	0.54
2:M:424:ASN:N	2:M:424:ASN:HD22	2.04	0.54
2:M:621:MET:CE	2:M:625:GLY:HA2	2.37	0.54
2:M:602:MET:CE	2:M:647:ILE:HD13	2.38	0.54
2:O:283:PRO:HD2	2:O:286:LYS:HB2	1.90	0.54
2:P:275:PRO:HD2	2:P:309:ARG:HD3	1.89	0.54
2:P:319:ASP:O	2:P:320:LEU:HB2	2.07	0.54
2:P:717:GLU:HG2	2:P:717:GLU:O	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD13	1:C:233:SER:HB3	1.89	0.54
1:D:432:SER:HA	1:D:555:ARG:HD3	1.90	0.54
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.90	0.54
2:N:583:CYS:HB3	2:N:586:THR:HG22	1.89	0.54
2:M:163:ALA:HB2	2:M:169:LEU:HG	1.90	0.54
2:O:497:ASP:OD1	2:O:523:GLU:HG3	2.08	0.54
2:P:248:ILE:HD12	5:P:1008:XE:XE	2.86	0.54
2:P:650:THR:HG22	9:P:1070:HOH:O	2.08	0.54
1:A:587:LYS:H	1:B:220:HIS:HE1	1.56	0.53
2:N:339:TYR:CD2	2:N:435:VAL:HG21	2.43	0.53
2:O:4:PHE:N	2:O:238:GLU:OE2	2.41	0.53
2:P:61:TYR:HD2	2:P:66:ARG:HD2	1.72	0.53
1:A:32:ALA:O	1:A:36:MET:HG2	2.08	0.53
1:B:416:ARG:HG3	1:B:416:ARG:NH1	2.22	0.53
1:C:102:VAL:HG11	5:C:1003[B]:XE:XE	2.84	0.53
2:P:426:ASN:O	2:P:427:TRP:HB2	2.08	0.53
1:A:620:LEU:HD21	5:A:1003[A]:XE:XE	2.85	0.53
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.24	0.53
1:C:281:HIS:ND1	1:C:282:GLY:N	2.57	0.53
2:N:613:ILE:O	2:N:671:PRO:HD3	2.07	0.53
2:O:523:GLU:OE2	2:O:656:LYS:HE2	2.09	0.53
1:B:510:LEU:N	1:B:510:LEU:CD1	2.72	0.53
1:D:98:VAL:HG13	1:D:610:VAL:HA	1.89	0.53
2:P:623:PRO:HA	2:P:707:THR:HA	1.90	0.53
2:M:87:ARG:HD2	9:M:1010:HOH:O	2.07	0.53
1:A:287:LEU:HD11	5:A:1010:XE:XE	2.86	0.53
1:C:640:VAL:CG1	1:C:644:LYS:HE3	2.39	0.53
1:D:299:GLU:HA	1:D:299:GLU:OE1	2.09	0.53
1:D:2:PRO:HA	9:D:1040:HOH:O	2.09	0.53
2:N:144:PHE:O	2:N:148:MET:HG3	2.08	0.53
2:P:341:GLU:OE2	2:P:427:TRP:CD1	2.61	0.53
1:C:118:ASN:OD1	1:C:209:HIS:HE1	1.92	0.53
2:O:491:ARG:HB2	2:O:491:ARG:NH1	2.22	0.53
2:O:686:SER:HB3	2:O:692:GLY:O	2.09	0.53
2:P:341:GLU:OE2	2:P:427:TRP:HD1	1.91	0.53
2:P:485:TYR:N	2:P:485:TYR:CD1	2.77	0.53
1:C:342:CYS:HA	1:C:367:TYR:CZ	2.44	0.53
1:A:414:SER:O	1:A:415:ASN:C	2.47	0.53
1:C:411:ARG:O	1:C:416:ARG:HG2	2.08	0.53
1:A:426:ARG:NH2	1:A:539:ILE:HB	2.25	0.52
2:M:424:ASN:H	2:M:424:ASN:ND2	2.07	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:527:LEU:HD13	2:N:598:PHE:HB3	1.91	0.52
2:P:322:ILE:HG21	2:P:434:ALA:HB1	1.91	0.52
2:O:233:THR:O	2:O:240:GLN:NE2	2.42	0.52
2:O:626:MET:HB3	2:O:630:THR:HB	1.91	0.52
1:D:332:THR:OG1	1:D:336:SER:OG	2.26	0.52
2:N:350:PHE:C	2:N:350:PHE:CD1	2.83	0.52
2:N:417:LEU:O	9:N:1164:HOH:O	2.19	0.52
2:O:434:ALA:O	2:O:437:LYS:HB2	2.09	0.52
1:C:633:ILE:HA	9:C:1074:HOH:O	2.09	0.52
2:N:156:GLU:HG2	5:N:1008:XE:XE	2.87	0.52
2:O:221:TYR:N	2:O:224:ARG:HH21	2.07	0.52
2:O:460:VAL:HG13	2:O:463:VAL:HG13	1.90	0.52
1:B:33:VAL:HG21	1:B:477:GLN:HE22	1.74	0.52
2:O:399:PHE:CE1	2:O:541:GLU:HG3	2.44	0.52
1:D:28:THR:HG21	1:D:33:VAL:HG12	1.91	0.52
1:D:559:LEU:HG	1:D:563:MET:HE2	1.92	0.52
2:P:585:TYR:CE1	2:P:656:LYS:HD3	2.45	0.52
1:A:96:THR:O	1:A:100:ARG:HG3	2.10	0.52
1:C:3:ARG:HH11	1:C:3:ARG:HG3	1.75	0.52
2:P:488:ARG:C	2:P:490:ASP:H	2.13	0.52
2:P:525:VAL:HB	9:P:1069:HOH:O	2.09	0.52
1:A:506:GLY:CA	1:A:511:LEU:HD12	2.39	0.52
2:O:136:ILE:HG21	2:O:221:TYR:CE2	2.45	0.52
2:O:549:GLN:HB3	2:O:550:PRO:CD	2.40	0.52
2:O:554:GLU:HG3	2:O:566:SER:HB3	1.90	0.52
2:O:657:PHE:HE2	2:O:667:ILE:HD11	1.75	0.52
1:B:577:VAL:HG12	1:B:601:PRO:HG2	1.92	0.52
1:C:396:SER:HB3	5:C:1010:XE:XE	2.88	0.52
1:C:500:CYS:HA	1:C:503:GLN:HG3	1.91	0.52
1:C:655:LYS:NZ	1:C:674:TYR:O	2.38	0.52
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.92	0.52
2:P:364:GLY:N	2:P:463:VAL:O	2.42	0.52
1:B:274:ASP:OD1	1:B:412:LYS:NZ	2.38	0.52
1:B:372:ILE:HD13	1:B:403:MET:HE3	1.92	0.52
2:O:356:VAL:HG11	2:O:360:GLU:OE2	2.10	0.52
2:P:142:ARG:HH11	2:P:142:ARG:HG2	1.75	0.52
2:P:333:ILE:HD12	2:P:418:TRP:HB2	1.92	0.52
2:P:681:GLU:CG	2:P:684:ARG:HH21	2.23	0.52
1:B:572:PRO:HG3	1:B:629:GLY:HA3	1.92	0.51
1:C:220:HIS:O	1:C:223:MET:HB2	2.11	0.51
1:C:563:MET:HE1	1:C:576:PHE:HD2	1.74	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.45	0.51
2:O:183:LEU:HB2	2:O:206:ALA:HA	1.93	0.51
2:O:351:GLU:HG3	2:O:423:ARG:HA	1.92	0.51
2:O:590:ASN:N	2:O:591:PRO:HD3	2.26	0.51
2:O:508:LEU:CB	3:O:900:SF4:S1	2.95	0.51
2:P:412:ASN:ND2	2:P:419:HIS:HB3	2.25	0.51
1:C:9:HIS:CD2	1:C:644:LYS:HG2	2.45	0.51
2:M:246:ARG:HE	2:M:247:ARG:NH1	2.08	0.51
2:N:408:HIS:HD2	2:N:419:HIS:ND1	2.08	0.51
2:O:382:LEU:HD23	2:O:469:THR:HG21	1.91	0.51
2:P:568:ASN:HD21	2:P:581:GLN:CG	2.22	0.51
1:C:114:CYS:HB2	1:C:208:ILE:HG21	1.92	0.51
2:M:95:ASN:HD21	2:M:98:ASN:H	1.57	0.51
1:D:191:ASN:ND2	9:D:1034:HOH:O	2.42	0.51
2:O:344:GLY:O	2:O:346:ARG:NH1	2.44	0.51
2:P:229:PHE:CD1	5:P:1009:XE:XE	3.41	0.51
1:B:256:PHE:CD1	1:B:289:GLU:HG3	2.46	0.51
1:D:292:VAL:HG11	1:D:326:GLN:HG3	1.93	0.51
1:C:611:GLU:HB2	9:C:1122:HOH:O	2.10	0.51
2:O:152:THR:O	2:O:154:PRO:HD3	2.11	0.51
2:O:224:ARG:O	2:O:228:MET:HB2	2.10	0.51
2:O:524:ARG:HB2	2:O:651:TYR:CE1	2.46	0.51
1:A:620:LEU:HD23	5:A:1004:XE:XE	2.88	0.51
2:O:254:TYR:CE2	2:O:258:HIS:CD2	2.98	0.51
2:O:430:VAL:HG11	2:O:439:PHE:CE2	2.45	0.51
2:P:343:GLY:O	2:P:346:ARG:NH1	2.43	0.51
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.93	0.51
2:N:335:LYS:HD3	2:N:429:ARG:HH12	1.76	0.51
2:O:277:ILE:N	2:O:277:ILE:HD12	2.25	0.51
2:P:340:VAL:HG13	2:P:341:GLU:N	2.26	0.51
2:O:612:MET:SD	2:O:622:THR:HB	2.51	0.51
2:P:385:GLY:O	2:P:467:ILE:HA	2.11	0.51
1:A:592:GLY:HA2	5:A:1001:XE:XE	2.89	0.51
1:B:394:ILE:HG23	1:B:395:GLU:H	1.76	0.51
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.93	0.51
2:O:26:TYR:CE1	2:O:30:ILE:HD11	2.46	0.51
1:A:220:HIS:HD2	1:A:221:MET:O	1.94	0.50
2:M:62:LEU:HD13	2:M:115:ALA:HB2	1.93	0.50
2:O:527:LEU:HA	2:O:648:GLY:N	2.26	0.50
2:P:403:LEU:N	2:P:403:LEU:HD23	2.26	0.50
2:P:564:TRP:HB2	2:P:567:VAL:HB	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:626:MET:SD	2:P:634:MET:HE3	2.52	0.50
1:D:266:ALA:HA	1:D:330:LEU:O	2.12	0.50
1:D:504:ALA:O	1:D:505:ALA:C	2.50	0.50
2:M:373:ILE:HG22	2:M:440:ARG:HD3	1.93	0.50
2:O:259:ASP:OD2	2:O:262:LYS:HD2	2.11	0.50
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.77	0.50
2:P:479:GLU:C	2:P:481:ALA:N	2.64	0.50
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.26	0.50
1:A:305:ALA:HB1	1:A:409:LYS:HD2	1.93	0.50
1:B:620:LEU:CD2	5:B:1004:XE:XE	3.38	0.50
2:O:269:ALA:HB1	2:O:274:PHE:HB2	1.93	0.50
2:P:358:GLU:HA	2:P:361:ILE:HG22	1.92	0.50
1:B:118:ASN:C	1:B:118:ASN:HD22	2.15	0.50
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.46	0.50
1:D:275:GLN:HG2	1:D:309:GLY:O	2.11	0.50
1:D:615:LEU:H	6:D:863:GOL:C1	2.25	0.50
2:M:373:ILE:HG21	2:M:439:PHE:O	2.11	0.50
2:M:95:ASN:C	2:M:95:ASN:HD22	2.15	0.50
2:N:679:HIS:HD2	2:N:680:ASP:OD1	1.94	0.50
1:B:620:LEU:HD22	5:B:1004:XE:XE	2.90	0.50
1:D:146:VAL:O	1:D:150:VAL:HG22	2.11	0.50
1:D:267:ASN:O	1:D:270:VAL:HG22	2.11	0.50
1:D:416:ARG:HB2	1:D:418:VAL:CG2	2.42	0.50
2:O:166:SER:HB3	2:O:192:GLN:HB3	1.93	0.50
2:O:362:THR:HB	2:O:365:LYS:HB2	1.94	0.50
2:O:392:GLY:HA2	2:O:461:ASP:HB2	1.93	0.50
2:O:725:MET:O	2:O:726:ASP:HB3	2.11	0.50
1:B:32:ALA:O	1:B:36:MET:HG2	2.11	0.50
1:D:41:LYS:O	1:D:41:LYS:HG2	2.12	0.50
2:P:602:MET:CE	2:P:645:MET:HE2	2.41	0.50
1:B:341:ILE:HA	1:B:346:ILE:HG12	1.93	0.50
1:C:202:ASN:HA	9:C:1120:HOH:O	2.11	0.50
2:N:272:THR:O	2:N:272:THR:HG22	2.11	0.50
1:B:549:SER:HB2	9:B:1019:HOH:O	2.12	0.49
2:O:497:ASP:HB2	2:O:656:LYS:NZ	2.28	0.49
2:O:597:CYS:SG	3:O:900:SF4:S3	3.10	0.49
2:P:353:VAL:HG13	2:P:388:VAL:HB	1.93	0.49
1:C:584:MET:O	1:D:71:CYS:HB2	2.11	0.49
2:M:426:ASN:HD22	2:M:426:ASN:C	2.16	0.49
2:N:602:MET:CE	2:N:647:ILE:HG21	2.42	0.49
2:O:144:PHE:O	2:O:148:MET:CG	2.49	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:163:ALA:HB2	2:O:255:LEU:HD13	1.92	0.49
2:O:504:TYR:OH	2:O:537:LYS:HG2	2.11	0.49
2:P:24:GLU:CD	9:P:1085:HOH:O	2.50	0.49
2:N:588:MET:CE	2:N:604:ILE:HG23	2.40	0.49
2:O:529:GLY:HA3	2:O:599:GLU:OE2	2.12	0.49
2:O:669:TRP:HD1	2:O:711:ILE:HG21	1.78	0.49
2:P:275:PRO:CD	2:P:309:ARG:HD3	2.42	0.49
2:P:391:TYR:CD2	2:P:462:ARG:NH1	2.78	0.49
2:P:403:LEU:HD22	2:P:456:PHE:CZ	2.48	0.49
2:P:525:VAL:HG11	2:P:650:THR:HG22	1.95	0.49
1:C:579:SER:HA	1:C:603:HIS:O	2.12	0.49
2:O:136:ILE:HG21	2:O:221:TYR:HE2	1.77	0.49
2:O:402:VAL:C	2:O:404:GLU:N	2.65	0.49
2:O:508:LEU:N	3:O:900:SF4:S2	2.84	0.49
1:D:317:CYS:O	1:D:321:GLU:HG2	2.11	0.49
1:C:220:HIS:HE1	1:D:587:LYS:H	1.61	0.49
2:M:373:ILE:CG2	2:M:440:ARG:HA	2.43	0.49
2:P:674:LEU:O	2:P:678:LEU:HD12	2.12	0.49
1:A:281:HIS:HB3	1:A:351:VAL:HG12	1.94	0.49
1:D:333:SER:HA	1:D:503:GLN:NE2	2.28	0.49
1:D:282:GLY:HA3	1:D:352:ASP:OD1	2.13	0.49
2:N:365:LYS:HB3	2:N:464:GLN:HG3	1.95	0.49
2:O:184:PHE:HB3	2:O:209:LEU:HD11	1.95	0.49
2:O:457:PRO:O	2:O:458:ALA:CB	2.60	0.49
2:P:472:ALA:O	2:P:476:GLU:HB2	2.13	0.49
2:N:221:TYR:CD1	2:N:221:TYR:C	2.86	0.49
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.13	0.49
2:O:579:LEU:HD22	2:O:593:THR:CG2	2.42	0.49
2:P:373:ILE:HD13	2:P:435:VAL:HG22	1.94	0.49
1:A:443:GLN:HB2	1:A:451:VAL:HG21	1.94	0.49
2:O:649:ARG:HA	2:O:652:ILE:HD12	1.94	0.49
2:P:261:VAL:HG12	5:P:1006:XE:XE	2.91	0.49
1:A:571:THR:OG1	1:A:572:PRO:HD3	2.13	0.49
1:C:52:PHE:CZ	1:C:474:LYS:HA	2.48	0.48
2:O:138:ASP:HB2	2:O:139:PRO:HD3	1.95	0.48
2:O:250:ALA:N	2:O:309:ARG:HE	2.10	0.48
2:O:416:GLY:O	2:O:430:VAL:HA	2.13	0.48
1:C:563:MET:CE	1:C:576:PHE:CD2	2.88	0.48
1:D:164:GLN:O	1:D:168[A]:GLU:HG3	2.12	0.48
2:M:245:ARG:O	2:M:245:ARG:HG3	2.11	0.48
2:O:316:ILE:CG2	2:O:454:GLU:OE1	2.61	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:354:ARG:HG2	2:P:484:LYS:NZ	2.28	0.48
2:P:605:LEU:HD11	2:P:624:SER:HA	1.95	0.48
2:O:19:VAL:O	2:O:22:PHE:HB2	2.13	0.48
2:O:66:ARG:O	2:O:66:ARG:HG3	2.12	0.48
2:P:170:ALA:O	2:P:174:LYS:HB2	2.13	0.48
2:P:667:ILE:O	2:P:699:ILE:HG12	2.13	0.48
2:P:681:GLU:HG3	2:P:684:ARG:NH2	2.28	0.48
1:B:587:LYS:HE3	4:B:800:XCC:S4	2.53	0.48
1:C:596:VAL:HG21	1:C:632:PHE:CE2	2.48	0.48
2:O:261:VAL:HG12	5:O:1006:XE:XE	2.91	0.48
2:P:343:GLY:HA3	2:P:349:ALA:CB	2.39	0.48
1:C:540:GLY:HA2	9:C:1136:HOH:O	2.13	0.48
2:O:345:ASN:C	2:O:348:PRO:HD3	2.34	0.48
2:O:449:VAL:O	2:O:449:VAL:CG1	2.62	0.48
2:O:657:PHE:CE2	2:O:667:ILE:HD11	2.48	0.48
2:P:585:TYR:CZ	2:P:656:LYS:HD3	2.49	0.48
2:M:716:GLU:HG3	2:M:723:LEU:HD12	1.95	0.48
2:O:7:ILE:HD12	2:O:245:ARG:HD2	1.96	0.48
2:P:350:PHE:CD1	2:P:351:GLU:N	2.82	0.48
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.79	0.48
2:M:621:MET:HE1	2:M:625:GLY:CA	2.44	0.48
2:O:215:ILE:HG21	5:O:1006:XE:XE	2.92	0.48
2:O:672:LYS:C	2:O:674:LEU:H	2.16	0.48
1:A:506:GLY:HA2	1:A:511:LEU:HD12	1.96	0.48
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.79	0.48
1:C:384:TYR:N	1:C:384:TYR:CD1	2.80	0.48
1:D:147:CYS:HB3	1:D:152:ILE:HB	1.95	0.48
2:O:229:PHE:CD1	5:O:1009:XE:XE	3.45	0.48
2:P:341:GLU:HG3	2:P:429:ARG:HB3	1.95	0.48
1:A:384:TYR:CD2	2:N:84:ASN:HB3	2.49	0.48
1:B:443:GLN:HB2	1:B:451:VAL:HG21	1.96	0.48
1:C:569:VAL:CG1	1:C:573:LYS:HD3	2.43	0.48
1:C:615:LEU:HD23	1:C:615:LEU:C	2.34	0.48
2:N:340:VAL:HG22	2:N:341:GLU:N	2.29	0.48
2:O:402:VAL:C	2:O:404:GLU:H	2.16	0.48
2:O:556:GLU:HG3	2:O:564:TRP:NE1	2.29	0.48
2:P:576:ASN:O	2:P:577:ARG:HB2	2.14	0.48
2:O:503:PHE:O	2:O:551:ILE:N	2.36	0.48
2:O:685:ARG:HA	2:O:688:GLU:HB2	1.95	0.48
2:P:117[A]:ARG:NH2	9:P:1051:HOH:O	2.47	0.48
2:P:602:MET:HE3	2:P:645:MET:HB3	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ILE:HG23	1:B:395:GLU:N	2.29	0.47
1:C:384:TYR:N	1:C:384:TYR:HD1	2.11	0.47
1:C:3:ARG:HG3	1:C:3:ARG:NH1	2.29	0.47
2:N:568:ASN:ND2	2:N:581:GLN:HE21	2.11	0.47
2:O:485:TYR:HA	2:O:489:ASP:HB2	1.95	0.47
2:P:665:ALA:O	2:P:720:HIS:HE1	1.97	0.47
1:B:241:ASP:OD1	1:B:245:GLU:OE2	2.31	0.47
1:B:426:ARG:NH2	9:B:1216:HOH:O	2.46	0.47
1:D:46:ILE:HD12	6:D:860:GOL:H31	1.95	0.47
2:O:335:LYS:HD2	2:O:336:GLY:N	2.28	0.47
1:A:267:ASN:O	1:A:270:VAL:HG22	2.13	0.47
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.45	0.47
1:D:118:ASN:HD22	1:D:118:ASN:C	2.17	0.47
2:N:244:GLN:HG3	2:N:272:THR:CG2	2.45	0.47
1:A:658:VAL:O	1:A:662:VAL:HG23	2.15	0.47
1:D:559:LEU:HG	1:D:563:MET:CE	2.44	0.47
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.24	0.47
2:P:354:ARG:HD2	2:P:355:THR:H	1.79	0.47
2:P:491:ARG:O	2:P:495:LEU:HD12	2.15	0.47
2:P:527:LEU:HA	2:P:648:GLY:N	2.30	0.47
1:D:114:CYS:CA	9:D:1050:HOH:O	2.62	0.47
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.49	0.47
2:O:295:VAL:CG1	2:O:301:ILE:HG12	2.45	0.47
2:O:376:ILE:HG21	2:O:382:LEU:HD11	1.97	0.47
2:O:418:TRP:CZ3	2:O:429:ARG:NE	2.82	0.47
2:P:479:GLU:C	2:P:481:ALA:H	2.16	0.47
1:A:177:LEU:HB2	1:A:180:GLU:CD	2.35	0.47
1:B:317:CYS:O	1:B:321:GLU:HG2	2.15	0.47
1:C:154:VAL:HG13	1:C:162:LEU:HD11	1.97	0.47
1:C:545:PHE:N	1:C:545:PHE:CD1	2.83	0.47
1:D:278:PHE:HB3	1:D:312:LEU:HD23	1.96	0.47
2:M:340:VAL:HG22	2:M:341:GLU:N	2.29	0.47
2:O:276:VAL:N	2:O:291:TRP:O	2.46	0.47
2:P:150:ASP:OD1	2:P:152:THR:CG2	2.62	0.47
2:P:412:ASN:OD1	2:P:418:TRP:HA	2.13	0.47
1:C:126:GLU:HG2	1:C:132:ALA:HB2	1.97	0.47
1:C:318:THR:O	1:C:322:VAL:HG22	2.15	0.47
1:C:43:ASP:O	1:C:44:LYS:HB2	2.15	0.47
1:D:52:PHE:CZ	1:D:474:LYS:HA	2.50	0.47
1:D:82:ASP:OD1	1:D:83:GLY:N	2.44	0.47
2:N:95:ASN:C	2:N:95:ASN:HD22	2.17	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:162:ARG:HG3	2:O:188:GLU:HB2	1.97	0.47
1:C:107:LEU:HD21	1:C:215:LEU:HB3	1.96	0.47
2:N:162:ARG:HB2	2:N:188:GLU:HB2	1.96	0.47
2:O:107:TRP:NE1	2:O:268:GLY:HA3	2.29	0.47
2:O:118:TYR:CD2	2:O:121:TYR:HB2	2.50	0.47
2:O:66:ARG:CZ	2:O:234:PRO:HG2	2.45	0.47
1:A:191:ASN:OD1	1:A:194:ARG:HG2	2.14	0.47
1:D:447:ASN:ND2	1:D:450:ARG:HB2	2.30	0.47
2:M:315:LYS:HG3	9:M:1153:HOH:O	2.14	0.47
2:O:563:ILE:HG12	2:O:583:CYS:SG	2.55	0.47
2:P:339:TYR:HB2	2:P:432:LYS:HA	1.96	0.47
1:C:292:VAL:HA	1:C:312:LEU:HD11	1.96	0.47
2:M:150:ASP:OD1	2:M:152:THR:CG2	2.62	0.47
2:M:341:GLU:HG3	2:M:429:ARG:HG2	1.97	0.47
2:M:675:LYS:NZ	2:M:699:ILE:O	2.40	0.47
2:P:354:ARG:HH21	2:P:356:VAL:HG11	1.73	0.47
1:A:287:LEU:HD13	1:A:388:TYR:CE1	2.50	0.47
1:D:182:GLU:OE2	1:D:199:ARG:HD3	2.15	0.47
1:D:373:THR:CG2	1:D:380:ILE:HD12	2.45	0.47
2:M:129:PRO:O	2:M:132:TRP:HB2	2.15	0.47
2:M:602:MET:HE2	2:M:647:ILE:HD13	1.96	0.47
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.96	0.47
2:O:86:LYS:HD3	2:O:86:LYS:HA	1.62	0.47
2:P:490:ASP:O	2:P:492:MET:N	2.48	0.47
1:B:400:ALA:HA	1:B:403:MET:HE2	1.94	0.46
1:C:223:MET:SD	1:D:353:VAL:HB	2.54	0.46
2:M:206:ALA:O	2:M:208:PRO:HD3	2.15	0.46
2:O:124:ASP:OD1	2:O:124:ASP:N	2.40	0.46
2:O:524:ARG:NH1	2:O:645:MET:HE3	2.30	0.46
1:C:279:VAL:HG22	1:C:313:VAL:HG23	1.96	0.46
1:D:30:ASP:HA	1:D:508:LEU:HD21	1.97	0.46
2:N:381:LYS:HB2	2:N:381:LYS:HE2	1.43	0.46
2:N:681:GLU:HB3	2:N:684:ARG:NH2	2.29	0.46
2:O:181:PHE:CE1	2:O:251:PHE:HE2	2.33	0.46
2:O:427:TRP:O	2:O:428:LEU:HB2	2.13	0.46
2:O:488:ARG:HB3	2:O:488:ARG:NH1	2.30	0.46
2:P:343:GLY:CA	2:P:349:ALA:HB3	2.40	0.46
1:B:607:MET:HG3	1:B:608:PRO:O	2.15	0.46
1:D:25:ARG:NH2	1:D:41:LYS:HB2	2.30	0.46
2:M:560:ILE:O	2:M:660:ALA:HB2	2.15	0.46
2:M:704:ILE:O	2:M:704:ILE:HD12	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MET:HG3	9:B:1052:HOH:O	2.14	0.46
1:D:129:GLU:OE2	1:D:164:GLN:NE2	2.49	0.46
1:D:477:GLN:O	1:D:478:ASP:HB2	2.15	0.46
2:M:383:PRO:HG3	2:M:471:GLU:HG2	1.98	0.46
2:M:408:HIS:CD2	2:M:419:HIS:ND1	2.78	0.46
2:N:211:ASN:ND2	9:N:1016:HOH:O	2.39	0.46
2:N:657:PHE:O	2:N:663:GLY:HA2	2.15	0.46
2:O:169:LEU:HD13	2:O:193:LEU:HD21	1.97	0.46
2:P:488:ARG:HG2	2:P:491:ARG:NH2	2.30	0.46
1:D:107:LEU:HD21	1:D:215:LEU:HB3	1.98	0.46
1:D:555:ARG:HG2	9:D:1045:HOH:O	2.15	0.46
2:N:283:PRO:HG2	2:N:286:LYS:HG3	1.96	0.46
2:N:693:GLU:CD	2:N:693:GLU:H	2.19	0.46
2:O:193:LEU:HD22	2:O:198:VAL:HG21	1.98	0.46
2:P:571:LEU:HD12	2:P:575:SER:HB3	1.97	0.46
1:B:87:ARG:HD3	1:B:91:GLY:O	2.16	0.46
1:D:145:GLU:OE1	1:D:145:GLU:HA	2.16	0.46
2:M:611:ILE:HD11	2:M:667:ILE:HG12	1.98	0.46
2:N:147:LYS:HB3	2:N:153:ILE:HD12	1.96	0.46
2:N:540:TYR:CE1	2:N:544:HIS:HA	2.51	0.46
2:O:333:ILE:HG13	2:O:418:TRP:HB2	1.98	0.46
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.97	0.46
2:P:288:ILE:O	2:P:289:PRO:C	2.54	0.46
2:P:553:LYS:HG2	2:P:564:TRP:NE1	2.30	0.46
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.81	0.46
1:B:661[A]:GLU:HG3	1:B:665[A]:ARG:HH21	1.80	0.46
1:B:7:LEU:HD11	2:N:164:LYS:HB2	1.97	0.46
2:N:681:GLU:HB3	2:N:684:ARG:HH21	1.80	0.46
2:O:354:ARG:HE	2:O:356:VAL:HG22	1.81	0.46
2:P:316:ILE:CG2	2:P:316:ILE:O	2.61	0.46
2:P:457:PRO:O	2:P:458:ALA:HB3	2.16	0.46
1:A:31:PRO:HB2	1:A:423:ILE:HD13	1.98	0.46
1:C:381:PRO:HB2	9:C:1104:HOH:O	2.15	0.46
1:C:316:CYS:N	1:C:503:GLN:HE22	2.13	0.46
1:C:637:ASP:OD1	1:C:640:VAL:HG23	2.16	0.46
2:N:64:VAL:HG13	2:N:111:GLU:OE2	2.16	0.46
2:O:247:ARG:O	2:O:512:PHE:CZ	2.69	0.46
2:O:158:ILE:HG22	2:O:252:VAL:HG13	1.97	0.46
2:P:609:ASN:OD1	2:P:728:ILE:HG22	2.15	0.46
2:P:674:LEU:HD22	2:P:674:LEU:O	2.15	0.46
1:B:466:LEU:HA	1:B:496:VAL:HG23	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:621:MET:HE3	2:N:622:THR:N	2.31	0.46
2:O:488:ARG:C	2:O:490:ASP:N	2.67	0.46
2:O:58:THR:HA	2:O:138:ASP:OD2	2.16	0.46
2:O:95:ASN:ND2	2:O:98:ASN:H	2.13	0.46
2:P:344:GLY:O	2:P:346:ARG:CZ	2.64	0.46
2:P:524:ARG:HH12	2:P:645:MET:HE1	1.80	0.46
2:P:61:TYR:CD2	2:P:66:ARG:HD2	2.48	0.46
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.96	0.45
1:D:241:ASP:C	1:D:241:ASP:OD1	2.54	0.45
2:M:21:LEU:HB2	2:M:286:LYS:HA	1.97	0.45
2:M:704:ILE:HD12	2:M:704:ILE:C	2.36	0.45
2:N:61:TYR:HD2	2:N:66:ARG:HD2	1.82	0.45
2:O:167:LYS:HD3	2:O:196:GLU:OE2	2.16	0.45
2:O:266:ALA:O	2:O:269:ALA:N	2.46	0.45
2:O:346:ARG:HB3	2:O:381:LYS:HD3	1.98	0.45
2:P:456:PHE:O	2:P:459:ILE:HB	2.15	0.45
1:A:287:LEU:HB3	9:A:1020:HOH:O	2.15	0.45
1:B:602:THR:HG23	5:B:1001:XE:XE	2.94	0.45
1:B:432:SER:HA	1:B:555:ARG:HD3	1.98	0.45
1:B:580:ALA:CB	5:B:1001:XE:XE	3.39	0.45
1:B:9:HIS:CE1	1:B:644:LYS:HB3	2.51	0.45
1:D:61:ILE:HG23	1:D:66:ILE:HD12	1.98	0.45
2:N:189:ALA:HA	2:N:192:GLN:HE21	1.80	0.45
2:O:611:ILE:O	2:O:668:VAL:HG22	2.16	0.45
2:P:538:ALA:O	2:P:542:ILE:HG23	2.16	0.45
1:C:256:PHE:CG	1:C:289:GLU:HG3	2.52	0.45
1:C:105:MET:CE	1:C:609:PRO:HD3	2.42	0.45
1:D:186:LEU:O	1:D:190:ILE:HG23	2.16	0.45
2:O:151:TRP:HA	2:O:151:TRP:CE3	2.51	0.45
2:O:216:VAL:O	2:O:219:ALA:HB3	2.16	0.45
2:O:505:SER:CB	2:O:570:TYR:HE2	2.28	0.45
2:O:609:ASN:O	2:O:666:ARG:NH1	2.50	0.45
2:P:344:GLY:O	2:P:346:ARG:NH1	2.50	0.45
1:A:569:VAL:HA	1:A:672:GLN:HE22	1.81	0.45
1:B:283:HIS:CE1	1:B:587:LYS:HZ3	2.34	0.45
1:C:531:LEU:HA	1:C:531:LEU:HD23	1.53	0.45
1:C:569:VAL:HB	1:C:573:LYS:HD3	1.98	0.45
1:D:127:MET:SD	1:D:127:MET:C	2.95	0.45
2:M:261:VAL:CG1	5:M:1006:XE:XE	3.42	0.45
2:M:602:MET:HE2	2:M:647:ILE:HG21	1.98	0.45
2:M:657:PHE:O	2:M:663:GLY:HA2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:367:GLU:HB2	9:N:1171:HOH:O	2.17	0.45
2:O:144:PHE:HB3	2:O:153:ILE:HD11	1.97	0.45
2:P:439:PHE:O	2:P:440:ARG:HD2	2.16	0.45
1:B:386:ILE:HD11	1:B:403:MET:CE	2.47	0.45
1:C:288:SER:O	1:C:292:VAL:HG23	2.15	0.45
1:C:587:LYS:NZ	4:C:800:XCC:S4	2.85	0.45
1:D:545:PHE:N	1:D:545:PHE:CD1	2.84	0.45
2:M:373:ILE:HG21	2:M:440:ARG:HA	1.99	0.45
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.81	0.45
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.47	0.45
2:O:183:LEU:HD23	2:O:183:LEU:HA	1.71	0.45
2:O:439:PHE:CG	2:O:440:ARG:N	2.84	0.45
2:P:611:ILE:O	2:P:668:VAL:HG22	2.16	0.45
1:B:308:LYS:HD3	1:B:308:LYS:HA	1.57	0.45
2:O:346:ARG:HH22	2:O:427:TRP:HZ2	1.64	0.45
1:A:72:MET:HG3	1:B:105:MET:HE1	1.98	0.45
1:D:32:ALA:CB	1:D:268:MET:HG3	2.45	0.45
1:D:285:PRO:C	1:D:287:LEU:N	2.69	0.45
1:D:530:ARG:HH11	1:D:530:ARG:CG	2.30	0.45
1:D:572:PRO:O	1:D:652:ARG:CZ	2.65	0.45
1:D:600:VAL:HA	1:D:601:PRO:HD3	1.89	0.45
2:N:254:TYR:O	2:N:278:THR:HA	2.17	0.45
2:N:354:ARG:HB3	2:N:484:LYS:HE2	1.98	0.45
2:O:316:ILE:CG2	2:O:316:ILE:O	2.64	0.45
2:O:590:ASN:OD1	2:O:640:GLN:NE2	2.50	0.45
2:P:369:ILE:HG21	2:P:468:PHE:HD2	1.82	0.45
2:P:665:ALA:O	2:P:720:HIS:CE1	2.70	0.45
1:C:154:VAL:O	1:C:154:VAL:HG12	2.17	0.45
1:C:241:ASP:OD1	1:C:245:GLU:OE2	2.34	0.45
1:D:241:ASP:OD1	1:D:245:GLU:OE2	2.34	0.45
1:D:614:ASP:H	6:D:863:GOL:H32	1.82	0.45
2:O:373:ILE:C	2:O:375:GLN:H	2.20	0.45
2:O:508:LEU:C	2:O:510:GLN:H	2.19	0.45
2:O:534:LEU:O	2:O:537:LYS:HB3	2.16	0.45
2:P:212:PHE:O	2:P:215:ILE:HG22	2.17	0.45
2:P:602:MET:HE3	2:P:645:MET:HE2	1.99	0.45
1:D:138:LYS:HG3	1:D:255:LEU:O	2.17	0.45
1:D:287:LEU:HD13	1:D:388:TYR:CE1	2.51	0.45
2:M:551:ILE:HG21	2:M:567:VAL:HG22	1.98	0.45
2:M:621:MET:HE1	2:M:625:GLY:HA2	1.97	0.45
2:N:79:LEU:HD22	2:N:112:ILE:HG12	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:488:ARG:HG2	2:P:491:ARG:HH22	1.82	0.45
2:M:184:PHE:C	2:M:185:ILE:HG13	2.36	0.44
2:O:483:GLU:HA	2:O:486:LYS:HB2	1.99	0.44
2:O:675:LYS:CA	2:O:696:ILE:HD11	2.46	0.44
1:C:316:CYS:SG	4:C:800:XCC:S3	3.11	0.44
1:D:105:MET:HG2	1:D:105:MET:H	1.56	0.44
2:M:621:MET:CE	9:M:1140:HOH:O	2.65	0.44
2:N:389:ASP:HB2	2:N:464:GLN:HB3	1.99	0.44
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.52	0.44
2:P:309:ARG:HB3	2:P:311:ILE:HG13	1.99	0.44
2:P:723:LEU:HA	2:P:723:LEU:HD23	1.50	0.44
1:B:380:ILE:HG22	1:B:381:PRO:O	2.18	0.44
2:N:622:THR:HB	2:N:623:PRO:HD2	1.99	0.44
2:P:352:LEU:HG	2:P:353:VAL:N	2.33	0.44
2:P:474:VAL:HG13	2:P:475:LYS:HG3	2.00	0.44
2:P:604:ILE:O	2:P:605:LEU:HD13	2.17	0.44
2:P:605:LEU:HA	2:P:605:LEU:HD12	1.75	0.44
1:A:559:LEU:HG	1:A:563:MET:HE2	1.98	0.44
1:A:89:ILE:HG12	1:B:52:PHE:HA	1.99	0.44
1:A:220:HIS:CE1	1:B:587:LYS:HG3	2.51	0.44
1:C:114:CYS:CA	9:C:1089:HOH:O	2.63	0.44
1:C:563:MET:HE3	1:C:574:VAL:HG11	2.00	0.44
2:P:655:LYS:HA	2:P:685:ARG:HH12	1.82	0.44
1:A:218:GLN:HE22	1:A:233:SER:CB	2.30	0.44
1:B:18:ARG:HH21	6:B:861:GOL:H2	1.83	0.44
1:D:620:LEU:CD2	5:D:1004:XE:XE	3.43	0.44
1:D:552:ASP:O	1:D:555:ARG:HB2	2.17	0.44
2:N:327:ALA:HB2	9:N:1172:HOH:O	2.17	0.44
1:A:549:SER:N	1:A:552:ASP:HB2	2.32	0.44
1:C:470:CYS:SG	1:C:588:ALA:HB2	2.58	0.44
1:D:431:TRP:O	1:D:547:MET:HG2	2.18	0.44
2:N:229:PHE:CE1	5:N:1009:XE:XE	3.49	0.44
2:N:558:ASP:OD1	2:N:558:ASP:C	2.56	0.44
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.48	0.44
2:P:138:ASP:N	2:P:139:PRO:CD	2.81	0.44
2:P:657:PHE:CE2	2:P:667:ILE:HD11	2.53	0.44
1:A:137:VAL:HG13	1:A:254:ILE:HG23	1.99	0.44
1:A:27:ARG:HB3	1:A:27:ARG:CZ	2.48	0.44
2:N:626:MET:HB3	2:N:630:THR:HB	1.99	0.44
2:O:191:GLU:O	2:O:195:GLU:HB2	2.18	0.44
2:P:373:ILE:HD13	2:P:435:VAL:CG2	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:602:MET:CE	2:P:645:MET:CE	2.96	0.44
1:B:386:ILE:HD11	1:B:403:MET:HE2	2.00	0.44
1:B:384:TYR:HD2	1:B:403:MET:SD	2.41	0.44
1:C:650:GLU:HA	1:C:653:THR:OG1	2.18	0.44
2:M:424:ASN:N	2:M:424:ASN:ND2	2.66	0.44
2:N:185:ILE:HD12	2:N:185:ILE:N	2.33	0.44
2:O:174:LYS:HA	9:O:1030:HOH:O	2.17	0.44
2:O:649:ARG:C	2:O:651:TYR:H	2.20	0.44
2:P:371:PRO:HD2	2:P:469:THR:HB	1.99	0.44
2:P:585:TYR:O	2:P:658:ILE:HA	2.17	0.44
2:O:491:ARG:HH11	2:O:491:ARG:CB	2.30	0.44
2:O:572:TYR:CE2	2:O:577:ARG:HB3	2.53	0.44
2:P:354:ARG:O	2:P:390:ILE:HG22	2.18	0.44
1:B:537:ILE:HA	1:B:537:ILE:HD13	1.94	0.43
1:C:287:LEU:HB3	9:C:1118:HOH:O	2.17	0.43
1:D:66:ILE:H	1:D:66:ILE:HG13	1.65	0.43
2:O:180:GLY:HA2	2:O:326:PRO:CG	2.48	0.43
2:O:356:VAL:HG23	2:O:361:ILE:HD12	2.00	0.43
2:O:6:LYS:O	2:O:9:GLU:HB2	2.18	0.43
2:P:674:LEU:HD13	2:P:678:LEU:HD11	2.00	0.43
1:A:342:CYS:HA	1:A:367:TYR:CZ	2.53	0.43
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.53	0.43
1:D:607:MET:HG3	1:D:608:PRO:O	2.18	0.43
1:D:615:LEU:H	6:D:863:GOL:H11	1.83	0.43
2:N:558:ASP:OD1	2:N:560:ILE:N	2.51	0.43
2:O:193:LEU:O	2:O:198:VAL:HG13	2.18	0.43
2:O:95:ASN:HD22	2:O:95:ASN:C	2.20	0.43
2:P:3:ASP:O	2:P:6:LYS:HB3	2.18	0.43
1:B:114[A]:CYS:HB3	1:B:208:ILE:HG21	1.99	0.43
1:D:275:GLN:HG2	1:D:309:GLY:C	2.39	0.43
1:D:261:PRO:HA	1:D:429:ALA:O	2.18	0.43
2:M:604:ILE:HG23	2:M:611:ILE:HG22	2.01	0.43
2:N:384:LEU:HA	2:N:468:PHE:O	2.18	0.43
2:O:270:ILE:O	2:O:271:PHE:C	2.55	0.43
2:O:361:ILE:HD13	2:O:391:TYR:CB	2.46	0.43
2:P:339:TYR:C	2:P:339:TYR:CD1	2.91	0.43
2:P:613:ILE:HD13	2:P:652:ILE:HG12	1.99	0.43
1:A:220:HIS:CD2	1:A:221:MET:O	2.71	0.43
1:A:567:LEU:HD12	1:A:574:VAL:HG22	2.01	0.43
1:B:287:LEU:HD12	1:B:388:TYR:CE1	2.54	0.43
1:D:322:VAL:O	1:D:326:GLN:HB2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:478:MET:HG3	2:N:478:MET:O	2.18	0.43
2:O:142:ARG:NH1	2:O:228:MET:HG2	2.33	0.43
2:O:334:ARG:O	2:O:335:LYS:C	2.57	0.43
2:P:541:GLU:H	2:P:541:GLU:HG2	1.54	0.43
1:A:272:ASP:C	1:A:272:ASP:OD1	2.56	0.43
1:B:415:ASN:O	1:B:415:ASN:CG	2.57	0.43
1:B:483:THR:HB	1:B:638:PRO:HB2	2.01	0.43
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.74	0.43
1:D:217:ASN:O	1:D:223:MET:HG3	2.18	0.43
1:D:531:LEU:HA	1:D:531:LEU:HD23	1.75	0.43
2:M:621:MET:HE2	2:M:625:GLY:HA2	1.99	0.43
2:N:315:LYS:CE	9:N:1162:HOH:O	2.67	0.43
2:O:289:PRO:C	2:O:291:TRP:H	2.21	0.43
2:O:491:ARG:O	2:O:495:LEU:HB2	2.19	0.43
2:P:221:TYR:CD1	2:P:221:TYR:C	2.91	0.43
1:A:238:ALA:O	1:A:241:ASP:HB3	2.19	0.43
1:C:223:MET:HG2	1:D:354:GLN:HA	2.01	0.43
1:C:559:LEU:O	1:C:563:MET:HG3	2.18	0.43
2:N:51:HIS:HB3	2:N:76:LEU:HD12	2.01	0.43
2:O:334:ARG:NH1	2:O:335:LYS:CG	2.82	0.43
2:P:369:ILE:HG21	2:P:468:PHE:CD2	2.54	0.43
1:A:394:ILE:HA	1:A:394:ILE:HD12	1.75	0.43
1:B:47:THR:HB	1:B:338:GLU:OE1	2.19	0.43
2:M:335:LYS:HG3	2:M:429:ARG:HH22	1.83	0.43
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.53	0.43
2:O:608:CYS:SG	2:O:712:LEU:HD12	2.58	0.43
2:P:701:ASP:O	2:P:702:GLU:C	2.57	0.43
1:A:283:HIS:CE1	4:A:800:XCC:S3	3.11	0.43
1:A:426:ARG:HH22	1:A:539:ILE:HB	1.82	0.43
1:B:484:VAL:O	1:B:488:LEU:HG	2.19	0.43
1:C:281:HIS:O	1:C:351:VAL:HA	2.18	0.43
1:C:436:LEU:HA	1:C:436:LEU:HD23	1.74	0.43
2:N:423:ARG:HB3	2:N:485:TYR:CE2	2.53	0.43
2:N:674:LEU:HD22	2:N:678:LEU:HG	2.00	0.43
2:N:85:ARG:HD2	9:N:1043:HOH:O	2.18	0.43
2:P:358:GLU:HA	2:P:361:ILE:CG2	2.49	0.43
2:P:412:ASN:HD21	2:P:419:HIS:HB3	1.82	0.43
1:A:576:PHE:C	1:A:576:PHE:CD1	2.93	0.43
1:C:87:ARG:HD3	1:C:91:GLY:O	2.19	0.43
2:M:419:HIS:HE1	2:M:421:GLY:O	2.02	0.43
2:M:428:LEU:N	2:M:428:LEU:CD1	2.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:263:THR:O	2:O:266:ALA:HB3	2.19	0.43
2:O:569:ASP:O	2:O:573:THR:HG23	2.18	0.43
2:P:199:LYS:HG2	2:P:204:TYR:CZ	2.54	0.43
1:A:549:SER:O	1:A:552:ASP:HB2	2.19	0.43
1:B:280:LEU:HD13	1:B:288:SER:HB2	2.01	0.43
1:D:124:LEU:HD12	1:D:255:LEU:HD21	2.00	0.43
2:P:378:GLU:O	2:P:380:SER:N	2.52	0.43
2:P:426:ASN:O	2:P:427:TRP:CB	2.67	0.43
2:P:602:MET:HE1	2:P:647:ILE:HG21	2.01	0.43
2:P:588:MET:HE3	2:P:604:ILE:HD13	1.98	0.43
1:A:110:ALA:HA	1:A:241:ASP:OD2	2.19	0.42
1:A:470:CYS:HB3	4:A:800:XCC:S2	2.59	0.42
1:B:317:CYS:HB3	9:B:1019:HOH:O	2.19	0.42
1:B:50:ASP:OD2	9:B:1055:HOH:O	2.21	0.42
1:C:420:ILE:O	1:C:421:PRO:C	2.56	0.42
1:D:279:VAL:CG1	1:D:315:ILE:CD1	2.84	0.42
2:M:55:TYR:HB3	2:M:56:PRO:HD2	2.00	0.42
2:M:623:PRO:HA	2:M:707:THR:HA	2.01	0.42
2:N:160:LEU:HD21	2:N:262:LYS:HG2	2.01	0.42
2:N:316:ILE:HD13	2:N:317:LYS:O	2.19	0.42
2:O:527:LEU:HA	2:O:648:GLY:H	1.84	0.42
2:P:182:MET:HB2	2:P:205:ILE:HG22	2.00	0.42
1:A:186:LEU:HD22	1:A:205:PRO:HD2	2.00	0.42
1:A:574:VAL:O	1:A:576:PHE:N	2.51	0.42
2:M:604:ILE:HG22	2:M:610:GLY:O	2.19	0.42
2:O:509:CYS:CB	2:O:595:CYS:SG	3.07	0.42
2:P:150:ASP:OD1	2:P:150:ASP:C	2.57	0.42
1:B:268:MET:HA	1:B:331:VAL:HG23	2.01	0.42
1:B:287:LEU:HA	1:B:388:TYR:CZ	2.55	0.42
1:B:654:TRP:HE1	2:N:195:GLU:CD	2.23	0.42
1:C:209:HIS:CD2	1:D:213:SER:OG	2.69	0.42
2:N:382:LEU:HA	2:N:382:LEU:HD12	1.88	0.42
2:O:160:LEU:HD13	2:O:215:ILE:HD13	2.02	0.42
2:O:79:LEU:N	2:O:80:PRO:CD	2.82	0.42
2:P:448:LEU:O	2:P:452:MET:HG2	2.20	0.42
1:A:453:ASN:ND2	1:A:566:ASP:HB3	2.34	0.42
1:B:467:ILE:O	1:B:497:ALA:HA	2.19	0.42
1:C:574:VAL:O	1:C:576:PHE:N	2.50	0.42
1:D:134:ASP:HB3	1:D:290:ILE:HD12	2.00	0.42
2:N:66:ARG:HD3	9:N:1029:HOH:O	2.19	0.42
2:O:174:LYS:HE2	2:O:323:ASN:ND2	2.34	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:430:VAL:HG12	2:O:434:ALA:HB3	2.01	0.42
2:O:468:PHE:HB2	2:O:474:VAL:CG2	2.41	0.42
2:P:315[A]:LYS:HD3	9:P:1080:HOH:O	2.19	0.42
2:P:323:ASN:HB2	2:P:415:GLU:OE1	2.19	0.42
2:P:589:GLU:O	2:P:590:ASN:C	2.58	0.42
1:A:162:LEU:HD23	1:A:162:LEU:HA	1.72	0.42
1:B:579:SER:HA	1:B:603:HIS:O	2.20	0.42
1:B:602:THR:CG2	5:B:1001:XE:XE	3.46	0.42
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.01	0.42
1:D:592:GLY:HA2	5:D:1001:XE:XE	2.98	0.42
2:M:448:LEU:HA	2:M:448:LEU:HD12	1.90	0.42
2:M:503:PHE:CG	2:M:521:THR:HG22	2.54	0.42
2:N:466:THR:HG21	2:N:468:PHE:CZ	2.55	0.42
2:O:114:GLU:HG3	2:O:216:VAL:HG12	2.01	0.42
2:O:397:ALA:HA	2:O:400:GLU:HG3	2.01	0.42
2:P:722:ALA:HA	2:P:725:MET:SD	2.60	0.42
1:A:106:ILE:HD11	5:A:1003[A]:XE:XE	2.98	0.42
1:A:515:ASN:HA	1:A:518:THR:HG23	2.02	0.42
1:D:292:VAL:HG22	1:D:312:LEU:HD13	2.01	0.42
1:D:400:ALA:HB2	5:D:1010:XE:XE	2.98	0.42
2:M:602:MET:HE1	2:M:647:ILE:HD13	2.01	0.42
2:N:107:TRP:CZ3	2:N:219:ALA:HB1	2.54	0.42
2:N:405:ARG:HD2	9:N:1219:HOH:O	2.18	0.42
2:O:470:ASP:O	2:O:474:VAL:HB	2.19	0.42
2:P:528:CYS:HB3	3:P:900:SF4:S3	2.59	0.42
2:P:668:VAL:HB	2:P:715:LEU:HD11	2.01	0.42
1:A:338:GLU:HB2	9:A:1023:HOH:O	2.20	0.42
1:B:637:ASP:HA	1:B:638:PRO:HD2	1.75	0.42
2:M:525:VAL:HG23	2:M:532:SER:HA	2.01	0.42
2:N:199:LYS:HD2	2:N:204:TYR:CE2	2.55	0.42
2:N:478:MET:O	2:N:482:ARG:HG3	2.20	0.42
2:O:182:MET:HG3	2:O:205:ILE:HG22	2.01	0.42
2:O:482:ARG:HH12	2:O:485:TYR:HE1	1.67	0.42
2:O:669:TRP:CD1	2:O:711:ILE:HG21	2.53	0.42
2:P:184:PHE:HD1	2:P:209:LEU:HD21	1.84	0.42
2:P:392:GLY:H	2:P:395:MET:HB2	1.84	0.42
2:P:400:GLU:C	2:P:402:VAL:H	2.21	0.42
1:A:2:PRO:HB2	1:A:651:TYR:CE2	2.55	0.42
1:B:287:LEU:HD13	1:B:388:TYR:CD1	2.54	0.42
1:B:572:PRO:CG	1:B:629:GLY:HA3	2.50	0.42
1:C:283:HIS:CD2	1:C:317:CYS:CB	3.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:243:TYR:CZ	2:N:247:ARG:HD3	2.54	0.42
2:N:26:TYR:CE1	2:N:30:ILE:HD11	2.55	0.42
2:O:118:TYR:CE2	2:O:121:TYR:CD2	3.08	0.42
1:B:587:LYS:NZ	4:B:800:XCC:S4	2.91	0.42
1:C:154:VAL:O	1:C:154:VAL:CG1	2.67	0.42
1:B:536:ASN:HD22	1:C:23:LYS:HB3	1.85	0.42
1:D:215:LEU:HD22	1:D:234:ALA:HA	2.02	0.42
1:D:496:VAL:HG11	1:D:547:MET:SD	2.60	0.42
2:M:64:VAL:HB	2:M:223:LEU:HD12	2.02	0.42
2:N:527:LEU:HD12	2:N:527:LEU:C	2.40	0.42
2:O:278:THR:O	2:O:294:SER:HA	2.20	0.42
1:A:414:SER:O	1:A:416:ARG:HD2	2.19	0.42
1:A:577:VAL:HG13	1:A:649:LEU:CD2	2.50	0.42
1:D:287:LEU:HA	1:D:388:TYR:OH	2.19	0.42
2:M:152:THR:O	2:M:154:PRO:HD3	2.20	0.42
2:O:220:ASN:C	2:O:224:ARG:HH21	2.24	0.42
2:O:338:MET:SD	2:O:341:GLU:HB2	2.60	0.42
2:O:628:PHE:O	2:O:632:ALA:N	2.39	0.42
2:O:712:LEU:HA	2:O:715:LEU:HB2	2.00	0.42
2:P:289:PRO:O	2:P:290:ASP:HB2	2.20	0.42
2:P:395:MET:SD	2:P:459:ILE:HG23	2.60	0.42
1:B:176:ARG:O	1:B:207:GLY:HA3	2.20	0.41
1:B:577:VAL:HG13	1:B:649:LEU:CD2	2.50	0.41
1:B:620:LEU:HD21	5:B:1003[A]:XE:XE	2.98	0.41
1:D:353:VAL:O	1:D:354:GLN:HB2	2.19	0.41
2:M:16:LYS:HD2	2:M:16:LYS:HA	1.37	0.41
2:N:43:ALA:O	2:N:47:TYR:HD2	2.03	0.41
2:O:504:TYR:HA	2:O:549:GLN:O	2.20	0.41
2:O:675:LYS:HG2	2:O:675:LYS:H	1.61	0.41
1:B:88:GLY:HA3	3:B:700:SF4:S3	2.60	0.41
1:C:603:HIS:HA	1:C:633:ILE:HB	2.01	0.41
2:M:357:SER:O	2:M:360:GLU:HB2	2.20	0.41
2:N:349:ALA:HA	2:N:384:LEU:O	2.20	0.41
2:N:549:GLN:NE2	2:N:570:TYR:OH	2.53	0.41
2:O:127:LEU:O	2:O:128:LEU:HD23	2.20	0.41
2:O:368:VAL:HG22	2:O:442:LYS:HB3	2.01	0.41
2:P:369:ILE:HG23	2:P:370:GLY:N	2.36	0.41
2:P:481:ALA:HB1	2:P:485:TYR:CZ	2.55	0.41
1:A:213:SER:CB	1:B:209:HIS:HD2	2.33	0.41
1:D:28:THR:HG21	1:D:33:VAL:CG1	2.51	0.41
2:O:500:VAL:HG22	2:O:501:ASP:H	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LYS:NZ	1:A:253:ASP:OD2	2.44	0.41
1:A:607:MET:HG3	1:A:608:PRO:O	2.21	0.41
1:C:144:LYS:HG2	1:C:154:VAL:HG11	2.02	0.41
2:M:586:THR:OG1	2:M:661:ASP:OD2	2.38	0.41
2:M:669:TRP:HA	2:M:700:ALA:O	2.20	0.41
2:N:615:THR:HG21	2:N:674:LEU:HG	2.02	0.41
2:O:335:LYS:HG3	2:O:336:GLY:H	1.85	0.41
2:O:683:VAL:O	2:O:686:SER:HB2	2.21	0.41
1:A:23:LYS:HE3	9:A:1176:HOH:O	2.20	0.41
1:C:348:ALA:HA	1:C:370:ARG:O	2.21	0.41
2:M:278:THR:O	2:M:294:SER:HA	2.21	0.41
2:N:223:LEU:HA	2:N:223:LEU:HD23	1.88	0.41
2:N:243:TYR:CE2	2:N:247:ARG:HD3	2.56	0.41
2:P:268:GLY:O	2:P:272:THR:HG22	2.21	0.41
1:A:277:ASN:HB2	1:A:345:ALA:O	2.20	0.41
1:A:560:LEU:HD22	1:A:600:VAL:HG21	2.02	0.41
1:B:574:VAL:HA	1:B:575:PRO:HD3	1.89	0.41
1:D:416:ARG:C	1:D:418:VAL:H	2.24	0.41
1:D:466:LEU:HG	1:D:467:ILE:N	2.34	0.41
2:N:87:ARG:HD2	9:N:1013:HOH:O	2.20	0.41
2:O:302:VAL:O	2:O:306:MET:HG3	2.20	0.41
2:O:79:LEU:O	2:O:80:PRO:C	2.57	0.41
2:P:358:GLU:HG3	2:P:462:ARG:NH1	2.36	0.41
1:A:125:VAL:HG23	1:A:167:GLY:HA3	2.02	0.41
1:A:235:ILE:HD11	5:A:1004:XE:XE	2.98	0.41
1:A:603:HIS:HA	1:A:633:ILE:O	2.20	0.41
1:B:447:ASN:O	1:B:450:ARG:HB3	2.21	0.41
1:C:332:THR:HG23	1:C:333:SER:N	2.36	0.41
1:D:573:LYS:HE2	1:D:671:CYS:O	2.21	0.41
2:M:395:MET:C	2:M:396:GLN:HG3	2.41	0.41
2:M:463:VAL:HG12	2:M:464:GLN:N	2.36	0.41
2:M:606:PRO:O	2:M:608:CYS:N	2.54	0.41
2:O:142:ARG:CZ	2:O:228:MET:HG2	2.50	0.41
2:O:245:ARG:HG3	2:O:245:ARG:O	2.16	0.41
2:O:335:LYS:CD	2:O:336:GLY:N	2.83	0.41
2:O:482:ARG:NH1	2:O:482:ARG:HA	2.35	0.41
2:O:527:LEU:HD12	2:O:528:CYS:N	2.36	0.41
2:P:393:ARG:CZ	2:P:393:ARG:HB3	2.49	0.41
2:P:3:ASP:HB2	9:P:1058:HOH:O	2.20	0.41
2:P:556:GLU:OE1	2:P:559:PRO:HG3	2.21	0.41
2:P:95:ASN:O	2:P:96:PHE:C	2.59	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:PHE:CG	1:B:289:GLU:HG3	2.56	0.41
1:B:353:VAL:O	1:B:354:GLN:HB2	2.19	0.41
1:B:14:SER:O	6:B:861:GOL:H12	2.21	0.41
2:N:150:ASP:OD1	2:N:150:ASP:C	2.59	0.41
2:N:607:GLU:HB3	9:N:1067:HOH:O	2.21	0.41
2:O:340:VAL:HG12	2:O:380:SER:O	2.19	0.41
2:O:342:MET:HG3	2:O:384:LEU:HD23	2.02	0.41
2:O:396:GLN:HB2	2:O:399:PHE:CD2	2.55	0.41
2:O:408:HIS:O	2:O:412:ASN:HB2	2.21	0.41
2:P:163:ALA:CB	2:P:169:LEU:HB2	2.50	0.41
2:P:424:ASN:ND2	2:P:485:TYR:HD2	2.19	0.41
1:A:90:CYS:O	1:B:357:MET:HG2	2.21	0.41
1:B:466:LEU:HA	1:B:496:VAL:O	2.21	0.41
1:C:439:LEU:HD21	1:C:531:LEU:HD13	2.03	0.41
1:D:9:HIS:C	1:D:9:HIS:CD2	2.93	0.41
2:M:651:TYR:O	2:M:654:SER:HB3	2.21	0.41
2:N:16:LYS:HB3	2:N:16:LYS:HE2	1.63	0.41
2:N:245:ARG:HD2	9:N:1137:HOH:O	2.21	0.41
2:O:79:LEU:HD22	2:O:112:ILE:HG12	2.03	0.41
2:P:230:GLY:HA3	2:P:243:TYR:CE2	2.56	0.41
2:P:64:VAL:HB	2:P:223:LEU:HD12	2.03	0.41
1:A:118:ASN:C	1:A:118:ASN:HD22	2.23	0.41
1:D:249:THR:O	1:D:250:ASP:C	2.58	0.41
2:M:182:MET:HG3	2:M:205:ILE:HG22	2.03	0.41
2:M:309:ARG:HD2	2:M:309:ARG:HA	1.82	0.41
2:N:61:TYR:CD2	2:N:66:ARG:HD2	2.56	0.41
2:O:151:TRP:HE3	2:O:151:TRP:HA	1.86	0.41
2:O:602:MET:HG2	2:O:611:ILE:HD12	2.03	0.41
2:O:627:THR:O	2:O:628:PHE:C	2.58	0.41
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.51	0.41
2:P:626:MET:CE	2:P:631:LEU:HD13	2.50	0.41
2:P:79:LEU:O	2:P:80:PRO:C	2.59	0.41
1:A:401:ILE:HG22	1:A:405:ILE:HD12	2.03	0.41
1:B:316:CYS:HB3	1:B:317:CYS:H	1.66	0.41
1:C:256:PHE:CD1	1:C:289:GLU:HG3	2.55	0.41
1:C:73:ALA:HB2	1:D:584:MET:HG3	2.03	0.41
2:N:146:ILE:HG22	9:N:1044:HOH:O	2.21	0.41
2:O:111:GLU:HB2	2:O:216:VAL:HG21	2.02	0.41
2:O:243:TYR:CE2	2:O:247:ARG:HD2	2.56	0.41
2:O:407:ILE:O	2:O:410:PHE:N	2.54	0.41
1:C:316:CYS:HB3	1:C:317:CYS:H	1.78	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:282:LEU:HA	2:M:283:PRO:HD2	1.86	0.40
2:N:353:VAL:HG22	2:N:388:VAL:HB	2.02	0.40
2:N:424:ASN:HD22	2:N:425:ILE:N	2.19	0.40
2:O:444:TYR:O	2:O:448:LEU:HG	2.20	0.40
2:O:639:THR:O	2:O:640:GLN:C	2.58	0.40
2:P:18:PRO:HB2	2:P:21:LEU:HB3	2.03	0.40
2:P:316:ILE:HA	2:P:316:ILE:HD12	1.94	0.40
2:P:478:MET:CE	2:P:482:ARG:HH21	2.34	0.40
1:A:68:CYS:HB2	1:A:97:ILE:CG2	2.46	0.40
1:B:127:MET:HA	1:B:132:ALA:HB3	2.03	0.40
1:B:299:GLU:O	1:B:303:LYS:HG3	2.21	0.40
1:C:261:PRO:HA	1:C:429:ALA:O	2.21	0.40
1:D:36:MET:CE	1:D:343:THR:HA	2.50	0.40
2:M:67:CYS:SG	2:M:223:LEU:HB3	2.61	0.40
2:M:655:LYS:HG2	2:M:685:ARG:NH1	2.36	0.40
2:N:206:ALA:O	2:N:208:PRO:HD3	2.21	0.40
2:N:607:GLU:CB	9:N:1067:HOH:O	2.69	0.40
2:O:343:GLY:O	2:O:346:ARG:NH1	2.55	0.40
2:O:51:HIS:HA	2:O:52:PRO:HD3	1.91	0.40
2:O:590:ASN:C	2:O:640:GLN:HE21	2.25	0.40
2:O:602:MET:O	2:O:644:PHE:HA	2.21	0.40
2:P:607:GLU:HB3	2:P:708:VAL:HG11	2.03	0.40
1:A:2:PRO:HD3	1:A:625:SER:CB	2.51	0.40
1:B:218:GLN:HE22	1:B:233:SER:CB	2.34	0.40
1:D:285:PRO:C	1:D:287:LEU:H	2.24	0.40
1:D:399:THR:O	1:D:403:MET:HG3	2.22	0.40
1:D:564:ALA:HB1	1:D:569:VAL:O	2.21	0.40
2:M:114:GLU:O	2:M:115:ALA:C	2.57	0.40
2:M:184:PHE:HB3	2:M:209:LEU:HD11	2.03	0.40
2:M:571:LEU:HA	2:M:571:LEU:HD23	1.91	0.40
2:M:95:ASN:C	2:M:95:ASN:ND2	2.74	0.40
2:O:317:LYS:HA	2:O:318:LEU:HD23	2.03	0.40
2:P:505:SER:CB	2:P:570:TYR:CE2	3.05	0.40
1:C:325:ARG:HH11	1:C:325:ARG:HD2	1.67	0.40
1:C:552:ASP:C	1:C:554:SER:N	2.74	0.40
1:C:483:THR:HB	1:C:638:PRO:HB2	2.03	0.40
1:D:287:LEU:HA	1:D:388:TYR:CZ	2.56	0.40
2:M:342:MET:HB3	2:M:382:LEU:O	2.21	0.40
2:N:694:ASP:O	2:N:695:PHE:C	2.59	0.40
2:O:649:ARG:HG2	2:O:674:LEU:HD11	2.03	0.40
2:P:201:GLY:HA2	9:P:1017:HOH:O	2.20	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:266:ALA:O	2:P:269:ALA:HB3	2.21	0.40
2:P:326:PRO:O	2:P:327:ALA:C	2.58	0.40
2:P:510:GLN:HA	2:P:513:ALA:O	2.22	0.40
2:P:602:MET:HE2	2:P:645:MET:HB3	2.03	0.40
1:C:122:HIS:CD2	9:C:1127:HOH:O	2.71	0.40
1:C:515:ASN:HD22	1:C:515:ASN:HA	1.71	0.40
1:C:596:VAL:HG21	1:C:632:PHE:CD2	2.56	0.40
1:D:271:LEU:O	1:D:420:ILE:HD13	2.22	0.40
2:N:4:PHE:O	2:N:7:ILE:HG12	2.20	0.40
2:O:169:LEU:HD12	2:O:193:LEU:HG	2.04	0.40
2:O:308:THR:O	2:O:309:ARG:C	2.58	0.40
2:P:277:ILE:N	2:P:277:ILE:HD12	2.37	0.40
2:P:399:PHE:CD1	2:P:399:PHE:N	2.88	0.40
2:P:604:ILE:HG22	2:P:643:GLY:O	2.20	0.40
2:P:627:THR:O	2:P:631:LEU:HB2	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	671/674 (100%)	637 (95%)	31 (5%)	3 (0%)	34	54
1	B	671/674 (100%)	638 (95%)	31 (5%)	2 (0%)	41	61
1	C	671/674 (100%)	636 (95%)	33 (5%)	2 (0%)	41	61
1	D	671/674 (100%)	632 (94%)	36 (5%)	3 (0%)	34	54
2	M	726/729 (100%)	678 (93%)	41 (6%)	7 (1%)	15	28
2	N	726/729 (100%)	692 (95%)	27 (4%)	7 (1%)	15	28
2	O	725/729 (100%)	592 (82%)	104 (14%)	29 (4%)	3	3
2	P	726/729 (100%)	622 (86%)	78 (11%)	26 (4%)	3	4

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5587/5612 (100%)	5127 (92%)	381 (7%)	79 (1%)	11	20

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	316	ILE
2	O	335	LYS
2	O	348	PRO
2	O	372	ASP
2	O	408	HIS
2	O	428	LEU
2	O	458	ALA
2	O	470	ASP
2	O	581	GLN
2	O	726	ASP
2	P	423	ARG
2	P	424	ASN
2	P	427	TRP
1	A	267	ASN
1	A	415	ASN
1	B	473	LEU
1	C	416	ARG
1	D	473	LEU
2	M	315	LYS
2	N	290	ASP
2	N	315	LYS
2	N	316	ILE
2	N	658	ILE
2	O	319	ASP
2	O	358	GLU
2	O	373	ILE
2	O	478	MET
2	O	650	THR
2	O	657	PHE
2	P	319	ASP
2	P	338	MET
2	P	359	SER
2	P	370	GLY
2	P	380	SER
2	P	474	VAL
2	P	480	VAL
2	P	491	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	228	MET
2	M	316	ILE
2	M	345	ASN
2	M	596	GLY
2	M	658	ILE
2	N	228	MET
2	O	123	PRO
2	O	154	PRO
2	O	187	ASP
2	O	290	ASP
2	O	527	LEU
2	O	556	GLU
2	P	187	ASP
2	P	346	ARG
2	P	360	GLU
2	P	449	VAL
2	P	489	ASP
1	C	354	GLN
2	M	187	ASP
2	N	187	ASP
2	N	596	GLY
2	O	338	MET
2	O	374	ASP
2	O	493	ARG
2	O	509	CYS
2	P	320	LEU
2	P	337	ASP
2	P	378	GLU
2	P	596	GLY
1	A	316	CYS
1	B	354	GLN
1	D	267	ASN
1	D	354	GLN
2	O	345	ASN
2	O	406	ARG
2	P	10	GLY
2	P	393	ARG
2	P	379	GLY
2	P	522	PRO
2	P	336	GLY
2	O	727	PRO
2	P	638	GLY



### 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	542/543 (100%)	513 (95%)	29 (5%)	22	42
1	B	542/543 (100%)	519 (96%)	23 (4%)	30	54
1	C	542/543 (100%)	504 (93%)	38 (7%)	15	29
1	D	542/543 (100%)	510 (94%)	32 (6%)	19	37
2	M	610/611 (100%)	556 (91%)	54 (9%)	9	19
2	N	610/611 (100%)	567 (93%)	43 (7%)	15	29
2	O	608/611 (100%)	489 (80%)	119 (20%)	1	2
2	P	610/611 (100%)	519 (85%)	91 (15%)	3	5
All	All	4606/4616 (100%)	4177 (91%)	429 (9%)	9	17

All (429) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	23	LYS
1	A	27	ARG
1	A	114	CYS
1	A	118	ASN
1	A	126	GLU
1	A	145	GLU
1	A	153	GLU
1	A	168	GLU
1	A	206	PHE
1	A	293	GLN
1	A	318	THR
1	A	331	VAL
1	A	336	SER
1	A	370	ARG
1	A	395	GLU
1	A	415	ASN
1	A	416	ARG
1	A	426	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	438	LYS
1	A	482	LEU
1	A	501	SER
1	A	518	THR
1	A	538	GLU
1	A	585	SER
1	A	647	ASP
1	A	656	LEU
1	A	664	GLU
1	A	665[A]	ARG
1	B	77	ARG
1	B	82[A]	ASP
1	B	114[A]	CYS
1	B	118	ASN
1	B	185	TRP
1	B	206	PHE
1	B	298	MET
1	B	336	SER
1	B	394	ILE
1	B	395	GLU
1	B	406	GLU
1	B	413	GLU
1	B	415	ASN
1	B	416	ARG
1	B	447	ASN
1	B	470	CYS
1	B	482	LEU
1	B	501	SER
1	B	518	THR
1	B	531	LEU
1	B	539	ILE
1	B	647	ASP
1	B	656	LEU
1	C	12	ARG
1	C	23	LYS
1	C	66	ILE
1	C	82	ASP
1	C	86	SER
1	C	114	CYS
1	C	118	ASN
1	C	185	TRP
1	C	196	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	206	PHE
1	C	218	GLN
1	C	233	SER
1	C	260	GLN
1	C	291	ILE
1	C	331	VAL
1	C	359	SER
1	C	360	ILE
1	C	370	ARG
1	C	384	TYR
1	C	411	ARG
1	C	412	LYS
1	C	413	GLU
1	C	416	ARG
1	C	438	LYS
1	C	470	CYS
1	C	482	LEU
1	C	501	SER
1	C	507	LYS
1	C	539[A]	ILE
1	C	546	HIS
1	C	579	SER
1	C	585	SER
1	C	600	VAL
1	C	647	ASP
1	C	653	THR
1	C	656	LEU
1	C	664	GLU
1	C	669	LYS
1	D	3	ARG
1	D	12	ARG
1	D	40	SER
1	D	66	ILE
1	D	77	ARG
1	D	82	ASP
1	D	105	MET
1	D	118	ASN
1	D	155	GLU
1	D	159	VAL
1	D	185	TRP
1	D	190	ILE
1	D	199	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	206	PHE
1	D	293	GLN
1	D	299	GLU
1	D	326	GLN
1	D	331	VAL
1	D	395	GLU
1	D	396	SER
1	D	470	CYS
1	D	482	LEU
1	D	496	VAL
1	D	517	GLU
1	D	518	THR
1	D	533	GLU
1	D	539	ILE
1	D	546	HIS
1	D	613	SER
1	D	647	ASP
1	D	656	LEU
1	D	664	GLU
2	M	6	LYS
2	M	16	LYS
2	M	17	GLU
2	M	66	ARG
2	M	95	ASN
2	M	127	LEU
2	M	152	THR
2	M	164	LYS
2	M	169	LEU
2	M	174	LYS
2	M	214	GLN
2	M	215	ILE
2	M	221	TYR
2	M	238[A]	GLU
2	M	245	ARG
2	M	254	TYR
2	M	284	GLU
2	M	315	LYS
2	M	317	LYS
2	M	334	ARG
2	M	335	LYS
2	M	342	MET
2	M	354	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	373	ILE
2	M	381	LYS
2	M	382	LEU
2	M	393	ARG
2	M	405	ARG
2	M	422	GLN
2	M	424	ASN
2	M	425	ILE
2	M	426	ASN
2	M	448	LEU
2	M	470	ASP
2	M	475	LYS
2	M	478	MET
2	M	479	GLU
2	M	486	LYS
2	M	539	SER
2	M	571	LEU
2	M	598	PHE
2	M	602	MET
2	M	604	ILE
2	M	621	MET
2	M	631	LEU
2	M	634	MET
2	M	672	LYS
2	M	674	LEU
2	M	686	SER
2	M	693	GLU
2	M	702	GLU
2	M	704	ILE
2	M	726	ASP
2	M	729	MET
2	N	14	GLU
2	N	66	ARG
2	N	95	ASN
2	N	152	THR
2	N	254	TYR
2	N	262	LYS
2	N	313	LEU
2	N	314	THR
2	N	315	LYS
2	N	316	ILE
2	N	317	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	N	334	ARG
2	N	335	LYS
2	N	342	MET
2	N	354	ARG
2	N	362	THR
2	N	373	ILE
2	N	396	GLN
2	N	405	ARG
2	N	424	ASN
2	N	425	ILE
2	N	437	LYS
2	N	440	ARG
2	N	442	LYS
2	N	448	LEU
2	N	451	LYS
2	N	462	ARG
2	N	470	ASP
2	N	475	LYS
2	N	478	MET
2	N	495	LEU
2	N	571	LEU
2	N	588	MET
2	N	598	PHE
2	N	604	ILE
2	N	606	PRO
2	N	631	LEU
2	N	639	THR
2	N	674	LEU
2	N	675	LYS
2	N	686	SER
2	N	704	ILE
2	N	729	MET
2	O	2	THR
2	O	3	ASP
2	O	5	ASP
2	O	7	ILE
2	O	14	GLU
2	O	16	LYS
2	O	17	GLU
2	O	19	VAL
2	O	34	SER
2	O	39	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	O	62	LEU
2	O	64	VAL
2	O	66	ARG
2	O	95	ASN
2	O	97	GLU
2	O	125	GLU
2	O	127	LEU
2	O	150	ASP
2	O	164	LYS
2	O	205	ILE
2	O	245	ARG
2	O	284	GLU
2	O	285	ASP
2	O	303	GLN
2	O	313	LEU
2	O	314	THR
2	O	318	LEU
2	O	320	LEU
2	O	323	ASN
2	O	332	SER
2	O	334	ARG
2	O	335	LYS
2	O	338	MET
2	O	340	VAL
2	O	342	MET
2	O	346	ARG
2	O	347	THR
2	O	350	PHE
2	O	352	LEU
2	O	354	ARG
2	O	356	VAL
2	O	357	SER
2	O	358	GLU
2	O	359	SER
2	O	361	ILE
2	O	362	THR
2	O	366	ILE
2	O	367	GLU
2	O	368	VAL
2	O	378	GLU
2	O	384	LEU
2	O	393	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	O	394	LYS
2	O	398	ASP
2	O	399	PHE
2	O	402	VAL
2	O	405	ARG
2	O	406	ARG
2	O	409	ASP
2	O	420	THR
2	O	425	ILE
2	O	426	ASN
2	O	427	TRP
2	O	428	LEU
2	O	429	ARG
2	O	440	ARG
2	O	451	LYS
2	O	461	ASP
2	O	463	VAL
2	O	465	VAL
2	O	466	THR
2	O	473	LYS
2	O	478	MET
2	O	482	ARG
2	O	485	TYR
2	O	487	GLU
2	O	489	ASP
2	O	490	ASP
2	O	491	ARG
2	O	492	MET
2	O	493	ARG
2	O	496	THR
2	O	497	ASP
2	O	523	GLU
2	O	524	ARG
2	O	534	LEU
2	O	535	ASP
2	O	544	HIS
2	O	559	PRO
2	O	565	LYS
2	O	567	VAL
2	O	575	SER
2	O	577	ARG
2	O	579	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
2	O	586	THR
2	O	594	SER
2	O	598	PHE
2	O	604	ILE
2	O	609	ASN
2	O	612	MET
2	O	614	THR
2	O	615	THR
2	O	617	ASP
2	O	621	MET
2	O	623	PRO
2	O	631	LEU
2	O	634	MET
2	O	639	THR
2	O	658	ILE
2	O	670	MET
2	O	675	LYS
2	O	681	GLU
2	O	687	VAL
2	O	689	GLU
2	O	693	GLU
2	O	704	ILE
2	O	708	VAL
2	O	712	LEU
2	O	728	ILE
2	P	9	GLU
2	P	39	LEU
2	P	64	VAL
2	P	66	ARG
2	P	95	ASN
2	P	96	PHE
2	P	125	GLU
2	P	130	PRO
2	P	146[A]	ILE
2	P	152	THR
2	P	174	LYS
2	P	182	MET
2	P	198	VAL
2	P	199	LYS
2	P	205	ILE
2	P	221	TYR
2	P	245	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	P	254	TYR
2	P	262	LYS
2	P	284	GLU
2	P	286	LYS
2	P	312	LYS
2	P	313	LEU
2	P	314	THR
2	P	316	ILE
2	P	331	GLU
2	P	334	ARG
2	P	335	LYS
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	351	GLU
2	P	354	ARG
2	P	355	THR
2	P	360	GLU
2	P	362	THR
2	P	365	LYS
2	P	369	ILE
2	P	373	ILE
2	P	382	LEU
2	P	388	VAL
2	P	390	ILE
2	P	393	ARG
2	P	398	ASP
2	P	409	ASP
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	431	SER
2	P	435	VAL
2	P	442	LYS
2	P	448	LEU
2	P	462	ARG
2	P	463	VAL
2	P	464	GLN
2	P	469	THR
2	P	473	LYS
2	P	474	VAL
2	P	485	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	P	486	LYS
2	P	487	GLU
2	P	490	ASP
2	P	491	ARG
2	P	493	ARG
2	P	498	GLU
2	P	501	ASP
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	551	ILE
2	P	556	GLU
2	P	563	ILE
2	P	565	LYS
2	P	569	ASP
2	P	571	LEU
2	P	579	LEU
2	P	598	PHE
2	P	605	LEU
2	P	631	LEU
2	P	639	THR
2	P	672	LYS
2	P	674	LEU
2	P	678	LEU
2	P	681	GLU
2	P	685	ARG
2	P	707	THR
2	P	717	GLU
2	P	718	LYS
2	P	726	ASP
2	P	728	ILE
2	P	729	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	209	HIS
1	A	217	ASN
1	A	218	GLN
1	A	220	HIS
1	A	260	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	471	ASN
1	A	477	GLN
1	A	503	GLN
1	A	515	ASN
1	A	622	GLN
1	A	672	GLN
1	B	56	GLN
1	B	58	GLN
1	B	122	HIS
1	B	209	HIS
1	B	217	ASN
1	B	218	GLN
1	B	220	HIS
1	B	454	GLN
1	B	471	ASN
1	B	477	GLN
1	B	503	GLN
1	B	515	ASN
1	B	622	GLN
1	B	672	GLN
1	C	56	GLN
1	C	58	GLN
1	C	209	HIS
1	C	217	ASN
1	C	218	GLN
1	C	220	HIS
1	C	293	GLN
1	C	368	HIS
1	C	471	ASN
1	C	477	GLN
1	C	503	GLN
1	C	515	ASN
1	C	622	GLN
1	D	56	GLN
1	D	58	GLN
1	D	209	HIS
1	D	217	ASN
1	D	218	GLN
1	D	220	HIS
1	D	454	GLN
1	D	471	ASN
1	D	477	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	503	GLN
1	D	515	ASN
1	D	622	GLN
2	M	95	ASN
2	M	192	GLN
2	M	211	ASN
2	M	408	HIS
2	M	424	ASN
2	M	426	ASN
2	M	510	GLN
2	M	581	GLN
2	M	590	ASN
2	N	95	ASN
2	N	192	GLN
2	N	211	ASN
2	N	408	HIS
2	N	424	ASN
2	N	510	GLN
2	N	549	GLN
2	N	581	GLN
2	N	590	ASN
2	N	679	HIS
2	O	95	ASN
2	O	192	GLN
2	O	211	ASN
2	O	258	HIS
2	O	323	ASN
2	O	396	GLN
2	O	516	HIS
2	O	568	ASN
2	O	578	ASN
2	O	590	ASN
2	O	640	GLN
2	P	27	HIS
2	P	95	ASN
2	P	192	GLN
2	P	211	ASN
2	P	303	GLN
2	P	396	GLN
2	P	424	ASN
2	P	426	ASN
2	P	510	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	P	515	ASN
2	P	568	ASN
2	P	576	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 75 ligands modelled in this entry, 50 are monoatomic - leaving 25 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	O	900	2	0,12,12	0.00	-	-		
6	GOL	C	861	-	5,5,5	0.59	0	5,5,5	0.78	0
6	GOL	B	863	-	5,5,5	0.77	0	5,5,5	1.63	2 (40%)
4	XCC	D	800	1	0,11,11	0.00	-	-		
3	SF4	D	700	1	0,12,12	0.00	-	-		
6	GOL	A	863	-	5,5,5	0.61	0	5,5,5	1.97	2 (40%)
6	GOL	C	860	-	5,5,5	0.52	0	5,5,5	0.65	0
3	SF4	C	700	1	0,12,12	0.00	-	-		
3	SF4	A	700	1	0,12,12	0.00	-	-		
3	SF4	C	750	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	D	863	-	5,5,5	0.84	0	5,5,5	1.33	1 (20%)
6	GOL	B	860	-	5,5,5	0.81	0	5,5,5	1.17	0
4	XCC	C	800	1	0,11,11	0.00	-	-		
4	XCC	A	800	1	0,11,11	0.00	-	-		
3	SF4	A	750	1	0,12,12	0.00	-	-		
6	GOL	D	860	-	5,5,5	0.52	0	5,5,5	0.37	0
6	GOL	A	861	-	5,5,5	0.70	0	5,5,5	1.30	1 (20%)
3	SF4	P	900	2	0,12,12	0.00	-	-		
3	SF4	B	700	1	0,12,12	0.00	-	-		
3	SF4	M	900	2	0,12,12	0.00	-	-		
4	XCC	B	800	1	0,11,11	0.00	-	-		
6	GOL	A	860	-	5,5,5	0.97	0	5,5,5	1.68	1 (20%)
6	GOL	B	861	-	5,5,5	0.69	0	5,5,5	0.97	0
3	SF4	N	900	2	0,12,12	0.00	-	-		
6	GOL	A	862	-	5,5,5	1.00	0	5,5,5	1.12	0

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	O	900	2	-	-	0/6/5/5
6	GOL	C	861	-	-	2/4/4/4	-
6	GOL	B	863	-	-	0/4/4/4	-
4	XCC	D	800	1	-	-	0/3/3/3
3	SF4	D	700	1	-	-	0/6/5/5
6	GOL	A	863	-	-	0/4/4/4	-
4	XCC	A	800	1	-	-	0/3/3/3
3	SF4	C	700	1	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
6	GOL	A	861	-	-	2/4/4/4	-
6	GOL	D	863	-	-	4/4/4/4	-
6	GOL	B	860	-	-	4/4/4/4	-
4	XCC	C	800	1	-	-	0/3/3/3
6	GOL	C	860	-	-	2/4/4/4	-
3	SF4	A	750	1	-	-	0/6/5/5
6	GOL	D	860	-	-	2/4/4/4	-
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
3	SF4	B	700	1	-	-	0/6/5/5

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	M	900	2	-	-	0/6/5/5
4	XCC	B	800	1	-	-	0/3/3/3
6	GOL	A	860	-	-	2/4/4/4	-
6	GOL	B	861	-	-	4/4/4/4	-
3	SF4	N	900	2	-	-	0/6/5/5
6	GOL	A	862	-	-	4/4/4/4	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	863	GOL	O3-C3-C2	-3.68	92.56	110.20
6	A	860	GOL	O1-C1-C2	2.84	123.80	110.20
6	D	863	GOL	O2-C2-C3	2.69	120.95	109.12
6	B	863	GOL	O2-C2-C1	-2.67	97.36	109.12
6	A	861	GOL	O3-C3-C2	2.56	122.46	110.20
6	B	863	GOL	O1-C1-C2	-2.31	99.13	110.20
6	A	863	GOL	C3-C2-C1	2.15	120.06	111.70

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	861	GOL	C1-C2-C3-O3
6	D	863	GOL	O1-C1-C2-C3
6	D	863	GOL	C1-C2-C3-O3
6	D	863	GOL	O2-C2-C3-O3
6	B	860	GOL	O1-C1-C2-C3
6	B	860	GOL	C1-C2-C3-O3
6	D	860	GOL	C1-C2-C3-O3
6	A	861	GOL	C1-C2-C3-O3
6	A	861	GOL	O2-C2-C3-O3
6	B	861	GOL	O1-C1-C2-C3
6	B	861	GOL	C1-C2-C3-O3
6	A	862	GOL	O1-C1-C2-O2
6	A	862	GOL	O1-C1-C2-C3
6	A	862	GOL	C1-C2-C3-O3
6	C	860	GOL	O2-C2-C3-O3
6	D	860	GOL	O2-C2-C3-O3
6	A	860	GOL	C1-C2-C3-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
6	C	860	GOL	C1-C2-C3-O3
6	C	861	GOL	O2-C2-C3-O3
6	A	860	GOL	O2-C2-C3-O3
6	B	860	GOL	O2-C2-C3-O3
6	B	861	GOL	O1-C1-C2-O2
6	B	861	GOL	O2-C2-C3-O3
6	A	862	GOL	O2-C2-C3-O3
6	B	860	GOL	O1-C1-C2-O2
6	D	863	GOL	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	O	900	SF4	5	0
6	C	861	GOL	1	0
6	B	863	GOL	2	0
4	D	800	XCC	1	0
6	D	863	GOL	6	0
4	C	800	XCC	3	0
4	A	800	XCC	2	0
6	D	860	GOL	1	0
6	A	861	GOL	1	0
3	P	900	SF4	1	0
3	B	700	SF4	1	0
4	B	800	XCC	3	0
6	B	861	GOL	3	0
6	A	862	GOL	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	673/674 (99%)	-0.39	11 (1%) 72 74	9, 18, 36, 61	2 (0%)
1	B	673/674 (99%)	-0.46	6 (0%) 84 86	8, 18, 35, 67	7 (1%)
1	C	673/674 (99%)	-0.44	4 (0%) 89 90	10, 23, 40, 61	3 (0%)
1	D	673/674 (99%)	-0.29	13 (1%) 66 69	11, 25, 46, 70	2 (0%)
2	M	728/729 (99%)	-0.43	4 (0%) 91 91	9, 25, 49, 70	4 (0%)
2	N	728/729 (99%)	-0.47	3 (0%) 92 93	7, 23, 48, 64	3 (0%)
2	O	727/729 (99%)	1.19	221 (30%) 0 0	24, 58, 90, 130	1 (0%)
2	P	728/729 (99%)	0.41	112 (15%) 2 1	12, 40, 84, 112	3 (0%)
All	All	5603/5612 (99%)	-0.10	374 (6%) 17 18	7, 25, 71, 130	25 (0%)

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	399	PHE	7.9
2	P	461	ASP	7.2
2	P	481	ALA	7.0
2	P	472	ALA	7.0
2	O	545	ALA	6.9
2	O	350	PHE	6.6
2	O	465	VAL	6.5
2	P	391	TYR	6.4
2	O	355	THR	6.4
2	M	314	THR	6.3
2	O	696	ILE	6.3
2	O	384	LEU	6.1
2	P	359	SER	6.0
2	P	458	ALA	6.0
2	O	490	ASP	6.0
2	O	692	GLY	5.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	O	314	THR	5.6
2	O	345	ASN	5.5
2	O	468	PHE	5.4
2	P	399	PHE	5.3
2	O	655	LYS	5.3
2	O	492	MET	5.3
2	O	460	VAL	5.3
2	O	380	SER	5.3
2	O	368	VAL	5.2
2	O	461	ASP	5.2
2	P	485	TYR	5.2
2	P	335	LYS	5.1
2	O	713	PRO	5.1
2	P	393	ARG	5.1
2	P	459	ILE	5.1
2	O	483	GLU	5.0
2	O	668	VAL	5.0
2	P	457	PRO	4.9
2	P	354	ARG	4.9
2	P	384	LEU	4.9
2	O	474	VAL	4.9
2	O	494	GLY	4.9
2	O	377	PRO	4.9
2	O	704	ILE	4.8
2	O	462	ARG	4.8
2	O	362	THR	4.8
2	O	344	GLY	4.8
2	O	473	LYS	4.7
2	O	479	GLU	4.7
2	P	364	GLY	4.7
2	O	582	VAL	4.7
2	P	362	THR	4.7
2	O	683	VAL	4.7
2	P	480	VAL	4.7
1	D	416	ARG	4.6
2	O	467	ILE	4.6
2	O	472	ALA	4.6
2	O	520	VAL	4.6
2	P	392	GLY	4.5
2	O	664	ILE	4.5
2	O	374	ASP	4.5
2	O	485	TYR	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	363	ASP	4.5
2	P	353	VAL	4.4
2	O	373	ILE	4.4
2	O	447	ILE	4.4
2	O	392	GLY	4.4
2	O	476	GLU	4.4
2	O	348	PRO	4.4
2	O	566	SER	4.3
2	O	573	THR	4.3
2	O	369	ILE	4.3
2	O	684	ARG	4.3
2	O	699	ILE	4.3
2	O	714	TYR	4.3
2	P	572	TYR	4.3
2	P	345	ASN	4.3
2	O	316	ILE	4.3
2	P	356	VAL	4.2
2	P	390	ILE	4.2
2	O	393	ARG	4.2
2	P	467	ILE	4.2
2	P	361	ILE	4.2
2	O	722	ALA	4.1
2	O	504	TYR	4.1
2	O	383	PRO	4.1
2	O	570	TYR	4.1
2	O	653	VAL	4.0
2	O	317	LYS	4.0
2	O	428	LEU	4.0
2	O	15	GLY	4.0
2	O	14	GLU	4.0
2	P	352	LEU	3.9
2	P	344	GLY	3.9
2	P	425	ILE	3.9
2	P	477	TYR	3.9
2	O	361	ILE	3.9
2	O	457	PRO	3.9
2	O	697	ASP	3.9
2	O	459	ILE	3.9
2	O	339	TYR	3.9
2	O	567	VAL	3.8
2	P	355	THR	3.8
2	P	729	MET	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	460	VAL	3.7
2	O	436	ALA	3.7
2	O	427	TRP	3.7
2	O	491	ARG	3.7
2	P	317	LYS	3.7
2	O	493	ARG	3.7
2	P	693	GLU	3.7
2	P	490	ASP	3.7
2	O	450	ALA	3.6
2	O	551	ILE	3.6
2	O	319	ASP	3.6
2	O	453	LYS	3.6
2	O	605	LEU	3.6
2	O	703	THR	3.6
1	B	539	ILE	3.6
2	P	398	ASP	3.6
2	O	391	TYR	3.6
2	P	387	LEU	3.6
2	O	470	ASP	3.6
2	O	550	PRO	3.6
2	O	533	TRP	3.6
2	O	662	GLY	3.6
2	O	559	PRO	3.5
2	O	425	ILE	3.5
2	O	695	PHE	3.5
2	O	363	ASP	3.5
2	P	696	ILE	3.5
2	O	544	HIS	3.5
2	P	492	MET	3.5
2	O	480	VAL	3.5
2	O	608	CYS	3.5
2	O	484	LYS	3.5
2	P	470	ASP	3.5
2	P	343	GLY	3.5
2	O	379	GLY	3.4
2	P	483	GLU	3.4
2	O	375	GLN	3.4
2	O	519	ILE	3.4
2	O	659	SER	3.4
2	O	548	ASN	3.4
2	O	469	THR	3.4
2	O	650	THR	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	O	718	LYS	3.4
2	P	692	GLY	3.3
2	O	572	TYR	3.3
2	P	338	MET	3.3
1	C	416	ARG	3.3
2	P	479	GLU	3.3
2	O	435	VAL	3.3
2	O	422	GLN	3.3
2	O	340	VAL	3.3
2	O	382	LEU	3.3
1	A	107	LEU	3.3
2	O	357	SER	3.3
2	P	623	PRO	3.3
2	P	488	ARG	3.3
2	O	564	TRP	3.3
2	P	476	GLU	3.2
1	A	416	ARG	3.2
2	O	463	VAL	3.2
2	O	540	TYR	3.2
2	O	663	GLY	3.2
2	N	729	MET	3.2
2	O	724	THR	3.2
2	O	395	MET	3.2
2	O	574	ALA	3.2
2	O	501	ASP	3.2
2	P	462	ARG	3.2
2	O	609	ASN	3.1
2	O	693	GLU	3.1
2	O	398	ASP	3.1
2	O	716	GLU	3.1
2	P	350	PHE	3.1
2	P	699	ILE	3.1
2	O	349	ALA	3.1
2	O	554	GLU	3.1
2	O	381	LYS	3.1
2	P	703	THR	3.1
2	P	493	ARG	3.1
1	A	415	ASN	3.1
2	O	705	GLY	3.1
2	P	394	LYS	3.1
2	O	372	ASP	3.0
1	C	230	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	2	THR	3.0
2	O	694	ASP	3.0
2	P	552	PRO	3.0
2	P	664	ILE	3.0
2	P	424	ASN	3.0
2	O	585	TYR	3.0
2	O	499	THR	3.0
2	O	502	THR	3.0
2	O	712	LEU	3.0
2	O	397	ALA	3.0
2	O	495	LEU	3.0
2	O	719	GLY	3.0
2	P	704	ILE	3.0
2	O	376	ILE	2.9
2	P	724	THR	2.9
1	B	538	GLU	2.9
2	P	570	TYR	2.9
2	O	386	ILE	2.9
2	O	690	GLY	2.9
2	P	358	GLU	2.9
2	O	583	CYS	2.9
2	P	473	LYS	2.9
2	O	389	ASP	2.8
2	P	542	ILE	2.8
2	P	469	THR	2.8
2	O	424	ASN	2.8
2	P	348	PRO	2.8
2	P	369	ILE	2.8
2	P	727	PRO	2.8
2	O	541	GLU	2.8
2	P	471	GLU	2.8
2	O	669	TRP	2.8
2	O	552	PRO	2.8
2	P	334	ARG	2.8
2	O	478	MET	2.8
2	O	522	PRO	2.8
2	P	491	ARG	2.8
2	O	400	GLU	2.8
1	A	106	ILE	2.8
2	O	394	LYS	2.8
2	P	504	TYR	2.8
2	P	389	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	P	395	MET	2.7
1	C	216	VAL	2.7
2	N	314	THR	2.7
2	O	542	ILE	2.7
2	O	665	ALA	2.7
2	O	682	PHE	2.7
2	P	569	ASP	2.7
2	P	342	MET	2.7
2	O	353	VAL	2.7
2	P	314	THR	2.7
2	O	560	ILE	2.7
2	P	581	GLN	2.7
2	O	418	TRP	2.7
2	O	315	LYS	2.6
2	O	482	ARG	2.6
2	O	723	LEU	2.6
2	O	672	LYS	2.6
2	O	612	MET	2.6
2	O	670	MET	2.6
2	O	356	VAL	2.6
2	O	725	MET	2.6
1	B	104	LEU	2.6
1	D	418	VAL	2.6
2	O	691	LEU	2.6
2	O	351	GLU	2.6
2	P	574	ALA	2.5
2	O	666	ARG	2.5
2	P	373	ILE	2.5
2	O	458	ALA	2.5
1	D	107	LEU	2.5
2	O	584	LEU	2.5
2	O	336	GLY	2.5
2	O	451	LYS	2.5
2	O	698	LYS	2.5
2	O	711	ILE	2.5
1	A	104	LEU	2.5
2	P	567	VAL	2.5
2	O	333	ILE	2.5
2	O	717	GLU	2.5
1	C	104	LEU	2.5
2	O	151	TRP	2.5
2	O	477	TYR	2.5

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	O	588	MET	2.4
2	O	727	PRO	2.4
2	O	678	LEU	2.4
2	O	347	THR	2.4
2	P	639	THR	2.4
2	P	698	LYS	2.4
1	D	415	ASN	2.4
2	P	610	GLY	2.4
2	P	565	LYS	2.4
2	O	2	THR	2.4
2	P	694	ASP	2.4
1	B	215	LEU	2.4
1	B	216	VAL	2.4
1	D	417	PRO	2.4
2	P	707	THR	2.4
2	O	364	GLY	2.4
2	O	555	GLY	2.4
2	P	486	LYS	2.4
2	O	657	PHE	2.4
2	O	676	ASP	2.4
2	O	530	ALA	2.4
2	O	487	GLU	2.3
2	O	359	SER	2.3
2	O	354	ARG	2.3
2	O	440	ARG	2.3
2	P	494	GLY	2.3
2	P	487	GLU	2.3
2	O	464	GLN	2.3
2	O	709	ASP	2.3
1	A	216	VAL	2.3
2	P	368	VAL	2.3
2	O	563	ILE	2.3
2	P	714	TYR	2.3
2	O	581	GLN	2.3
2	P	6	LYS	2.3
2	P	374	ASP	2.3
1	D	368	HIS	2.3
2	O	497	ASP	2.3
2	P	474	VAL	2.3
1	D	109	GLY	2.3
2	O	488	ARG	2.2
2	O	576	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	O	486	LYS	2.2
2	O	343	GLY	2.2
2	P	541	GLU	2.2
2	O	679	HIS	2.2
1	A	586	GLY	2.2
2	M	470	ASP	2.2
2	O	385	GLY	2.2
2	O	341	GLU	2.2
2	M	729	MET	2.2
2	O	577	ARG	2.2
1	D	413	GLU	2.2
2	M	713	PRO	2.2
2	P	691	LEU	2.2
2	O	557	ILE	2.2
2	P	14	GLU	2.2
2	P	705	GLY	2.2
2	O	687	VAL	2.2
2	O	688	GLU	2.2
2	P	721	PRO	2.2
2	O	580	GLU	2.2
2	O	388	VAL	2.2
2	P	463	VAL	2.2
2	O	429	ARG	2.2
2	O	565	LYS	2.1
2	O	420	THR	2.1
2	O	586	THR	2.1
2	P	573	THR	2.1
1	A	99	ALA	2.1
2	O	549	GLN	2.1
2	O	715	LEU	2.1
2	P	640	GLN	2.1
2	O	396	GLN	2.1
2	O	667	ILE	2.1
1	D	104	LEU	2.1
2	P	501	ASP	2.1
2	O	16	LYS	2.1
2	O	455	GLU	2.1
2	O	610	GLY	2.1
1	D	44	LYS	2.1
1	A	108	THR	2.1
1	D	108	THR	2.1
2	P	560	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	408	PHE	2.1
2	O	387	LEU	2.1
2	P	554	GLU	2.1
2	N	475	LYS	2.1
2	P	453	LYS	2.1
1	A	590	ALA	2.0
1	B	108	THR	2.0
1	D	216	VAL	2.0
2	P	708	VAL	2.0
2	O	358	GLU	2.0
2	O	640	GLN	2.0
2	O	338	MET	2.0
2	O	342	MET	2.0
1	A	538	GLU	2.0
2	O	707	THR	2.0
2	O	561	LYS	2.0
2	O	431	SER	2.0
2	O	449	VAL	2.0
2	P	668	VAL	2.0
2	O	456	PHE	2.0
2	P	468	PHE	2.0
2	P	396	GLN	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
6	GOL	C	861	6/6	0.73	0.18	53,59,59,60	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	B	861	6/6	0.78	0.30	45,51,52,54	0
6	GOL	A	861	6/6	0.81	0.28	34,47,51,53	0
6	GOL	D	863	6/6	0.87	0.23	28,36,42,42	0
6	GOL	D	860	6/6	0.87	0.17	47,51,52,52	0
7	CU1	O	950	1/1	0.90	0.04	88,88,88,88	0
6	GOL	C	860	6/6	0.90	0.15	39,48,50,51	0
4	XCC	D	800	9/9	0.91	0.13	52,61,69,69	0
5	XE	B	1001	1/1	0.92	0.41	32,32,32,32	1
6	GOL	B	860	6/6	0.93	0.12	27,27,30,30	0
5	XE	C	1001	1/1	0.94	0.27	13,13,13,13	1
4	XCC	B	800	9/9	0.94	0.12	37,52,54,57	0
4	XCC	C	800	9/9	0.94	0.11	40,54,66,66	0
4	XCC	A	800	9/9	0.95	0.11	37,48,56,57	0
5	XE	P	1008	1/1	0.95	0.29	19,19,19,19	1
6	GOL	A	863	6/6	0.95	0.17	22,26,32,35	0
3	SF4	O	900	8/8	0.96	0.05	59,60,62,62	0
5	XE	O	1007	1/1	0.96	0.15	33,33,33,33	1
7	CU1	P	950	1/1	0.96	0.05	52,52,52,52	0
6	GOL	B	863	6/6	0.96	0.17	30,34,37,37	0
6	GOL	A	862	6/6	0.96	0.17	27,30,35,35	0
5	XE	N	1008	1/1	0.97	0.20	25,25,25,25	1
5	XE	M	1006	1/1	0.97	0.15	29,29,29,29	1
5	XE	D	1001	1/1	0.97	0.11	34,34,34,34	1
5	XE	A	1003[A]	1/1	0.98	0.20	30,30,30,30	1
5	XE	A	1003[B]	1/1	0.98	0.20	14,14,14,14	1
7	CU1	M	950	1/1	0.98	0.10	30,30,30,30	0
8	NI	O	951	1/1	0.98	0.04	75,75,75,75	0
5	XE	D	1010	1/1	0.98	0.13	25,25,25,25	1
5	XE	N	1006	1/1	0.98	0.13	27,27,27,27	1
6	GOL	A	860	6/6	0.98	0.10	17,20,23,27	0
5	XE	O	1006	1/1	0.99	0.30	30,30,30,30	1
5	XE	C	1003[A]	1/1	0.99	0.15	29,29,29,29	1
3	SF4	C	750	8/8	0.99	0.07	22,26,28,28	0
5	XE	D	1003[A]	1/1	0.99	0.22	28,28,28,28	1
5	XE	O	1009	1/1	0.99	0.09	42,42,42,42	1
5	XE	C	1010	1/1	0.99	0.07	35,35,35,35	1
5	XE	D	1003[B]	1/1	0.99	0.22	30,30,30,30	1
5	XE	A	1010	1/1	0.99	0.03	31,31,31,31	1
5	XE	B	1010	1/1	0.99	0.07	24,24,24,24	1
3	SF4	P	900	8/8	0.99	0.05	31,34,36,37	0
5	XE	D	1004	1/1	0.99	0.14	28,28,28,28	1
5	XE	A	1002	1/1	0.99	0.12	27,27,27,27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SF4	B	700	8/8	0.99	0.12	7,9,11,15	0
8	NI	M	951	1/1	0.99	0.08	18,18,18,18	0
5	XE	C	1005	1/1	0.99	0.13	31,31,31,31	1
8	NI	P	951	1/1	0.99	0.06	44,44,44,44	0
5	XE	B	1003[B]	1/1	0.99	0.14	25,25,25,25	1
3	SF4	M	900	8/8	0.99	0.08	13,14,17,20	0
5	XE	B	1003[A]	1/1	0.99	0.14	26,26,26,26	1
5	XE	P	1006	1/1	0.99	0.20	29,29,29,29	1
5	XE	C	1002	1/1	0.99	0.10	33,33,33,33	0
3	SF4	C	700	8/8	0.99	0.10	21,23,24,24	0
5	XE	M	1008	1/1	0.99	0.14	30,30,30,30	1
3	SF4	D	700	8/8	0.99	0.11	18,19,20,22	0
3	SF4	A	700	8/8	0.99	0.12	10,12,14,14	0
7	CU1	N	950	1/1	0.99	0.12	28,28,28,28	0
5	XE	C	1003[B]	1/1	0.99	0.15	33,33,33,33	1
5	XE	A	1001	1/1	0.99	0.18	23,23,23,23	1
3	SF4	N	900	8/8	0.99	0.09	12,14,16,17	0
3	SF4	A	750	8/8	0.99	0.08	12,15,16,17	0
5	XE	D	1005	1/1	1.00	0.10	27,27,27,27	0
5	XE	M	1007	1/1	1.00	0.12	27,27,27,27	0
8	NI	N	951	1/1	1.00	0.09	17,17,17,17	0
5	XE	B	1005	1/1	1.00	0.10	21,21,21,21	0
5	XE	N	1007	1/1	1.00	0.11	21,21,21,21	0
5	XE	P	1007	1/1	1.00	0.11	29,29,29,29	0
5	XE	N	1009	1/1	1.00	0.13	34,34,34,34	1
5	XE	A	1005	1/1	1.00	0.10	24,24,24,24	0
5	XE	B	1004	1/1	1.00	0.11	29,29,29,29	1
5	XE	C	1004	1/1	1.00	0.14	30,30,30,30	1
5	XE	P	1009	1/1	1.00	0.15	31,31,31,31	1
5	XE	A	1004	1/1	1.00	0.10	30,30,30,30	1
5	XE	D	1002	1/1	1.00	0.15	29,29,29,29	1
5	XE	B	1002	1/1	1.00	0.12	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.