



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:11 AM EDT

PDB ID : 3I01 / pdb_00003i01
Title : Native structure of bifunctional carbon monoxide dehydrogenase/acetyl-CoA synthase from Moorella thermoacetica, water-bound C-cluster.
Authors : Kung, Y.; Doukov, T.I.; Drennan, C.L.
Deposited on : 2009-06-24
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

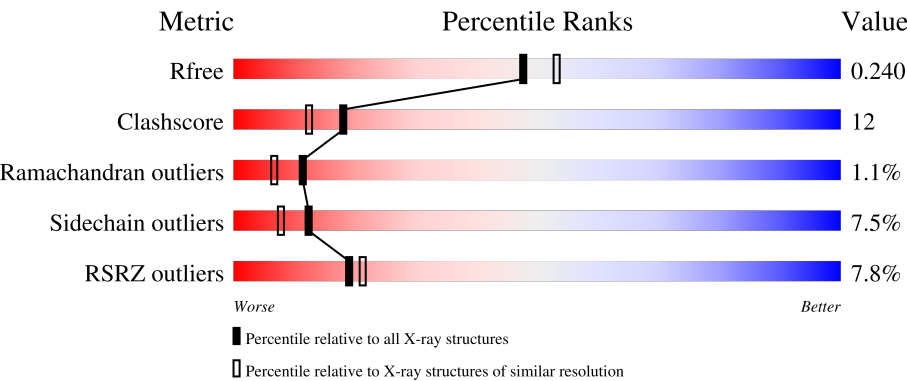
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	81%18%.
1	B	674	% 80%17%.
1	C	674	79%19%.
1	D	674	77%21%.
2	M	729	3% 76%20%. .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	O	900	-	-	X	-
4	XCC	D	800	-	-	X	-
5	GOL	C	863	-	-	X	-
5	GOL	D	863	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 45096 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

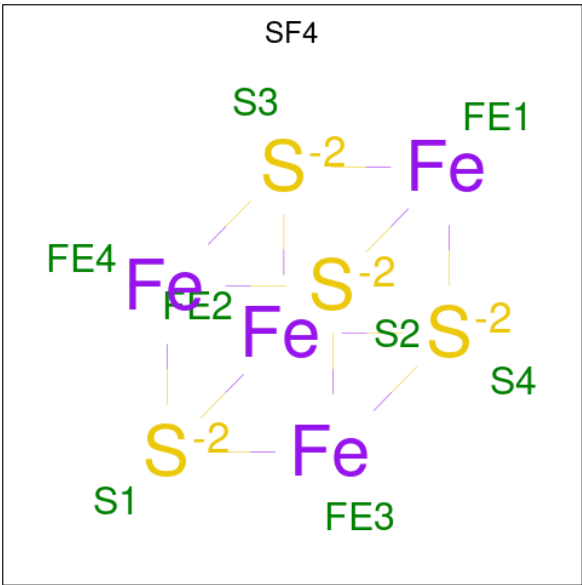
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

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

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

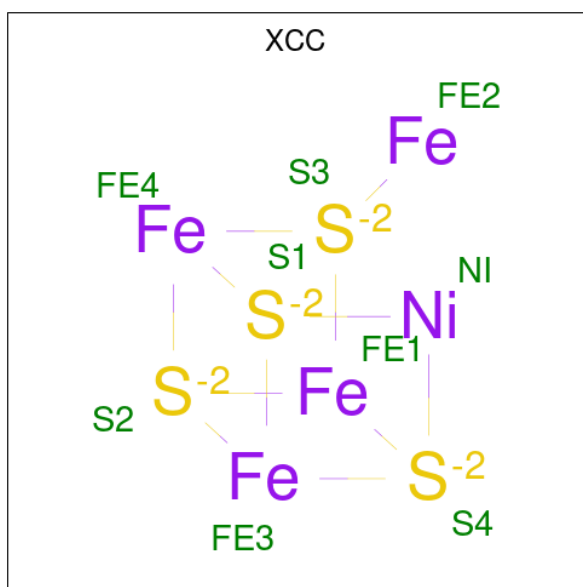
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	5	0
			5778	3703	964	1076	35			
2	N	728	Total	C	N	O	S	0	6	0
			5784	3707	968	1074	35			
2	O	728	Total	C	N	O	S	0	1	0
			5749	3687	958	1069	35			
2	P	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			

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



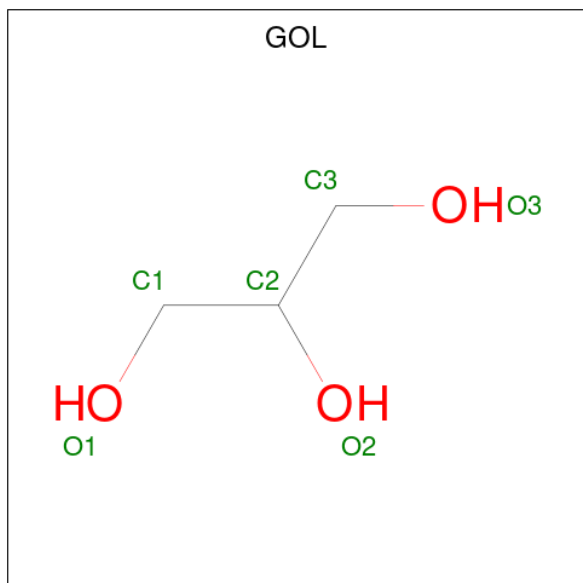
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3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

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



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

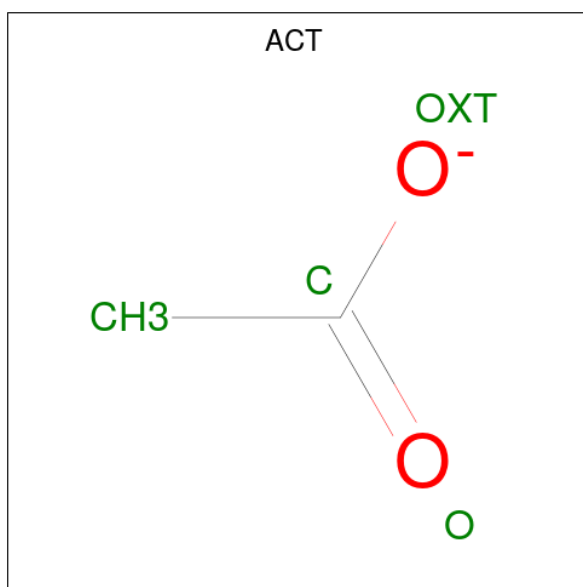
- Molecule 6 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

- Molecule 7 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 10 is water.

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

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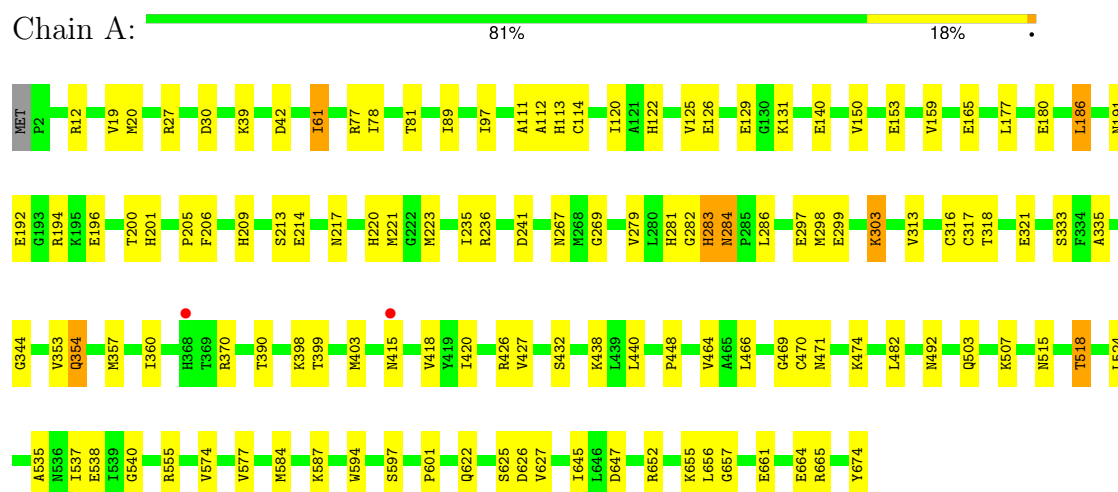
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	288	Total 288	O 288	0	0
10	C	169	Total 169	O 169	0	0
10	D	151	Total 151	O 151	0	0
10	M	218	Total 218	O 218	0	0
10	N	227	Total 227	O 227	0	0
10	O	27	Total 27	O 27	0	0
10	P	118	Total 118	O 118	0	0

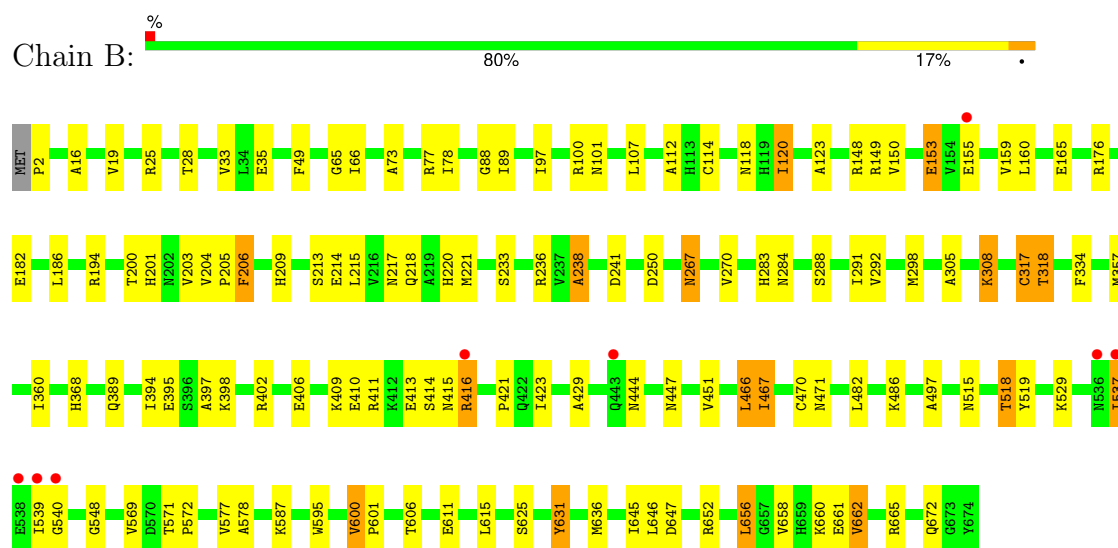
3 Residue-property plots

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

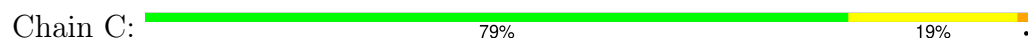
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

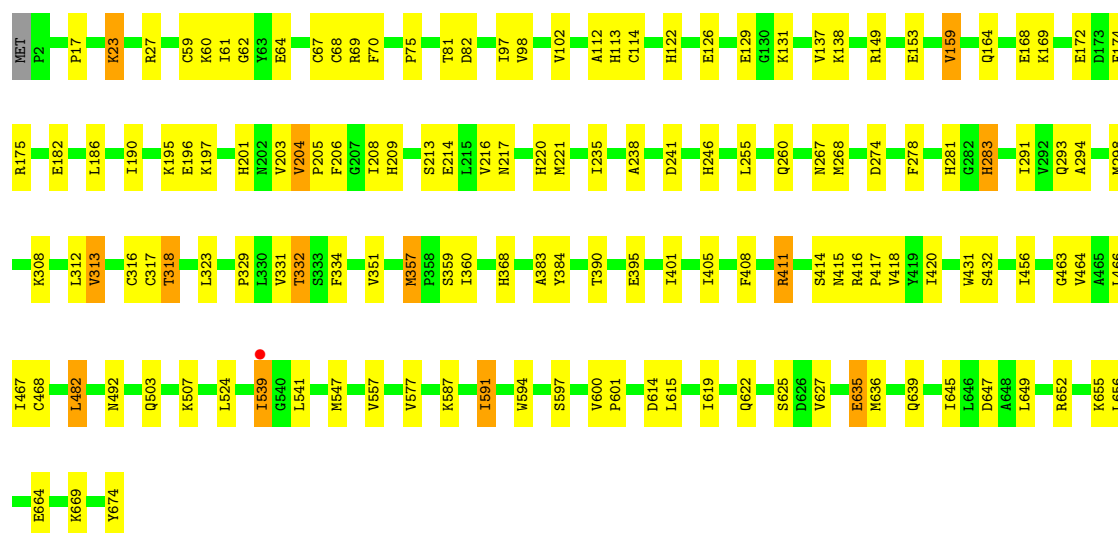


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



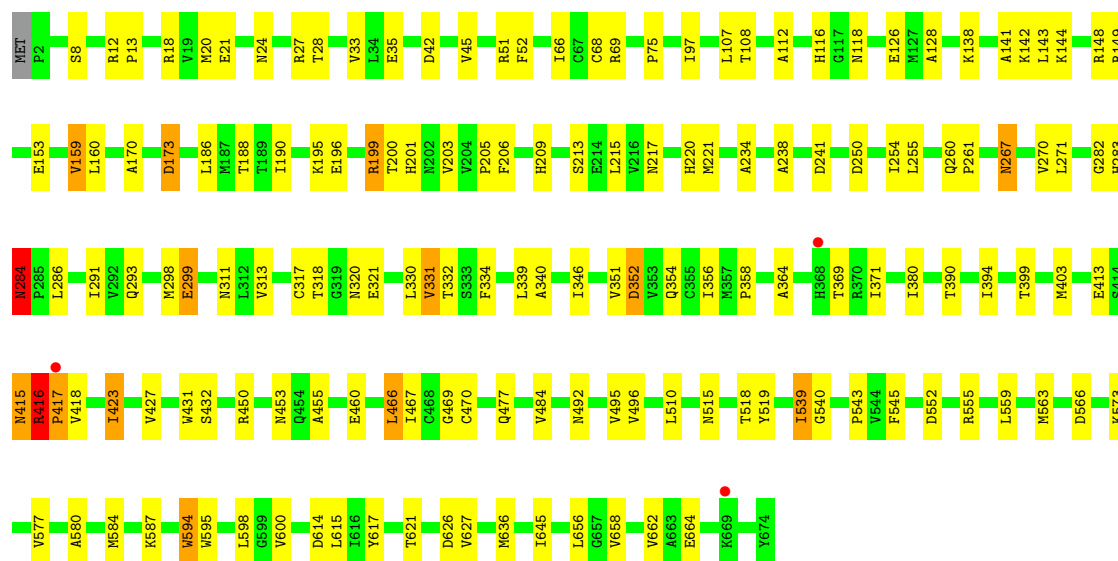
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta





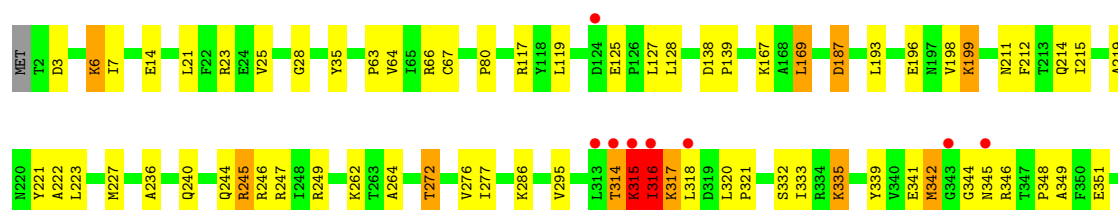
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

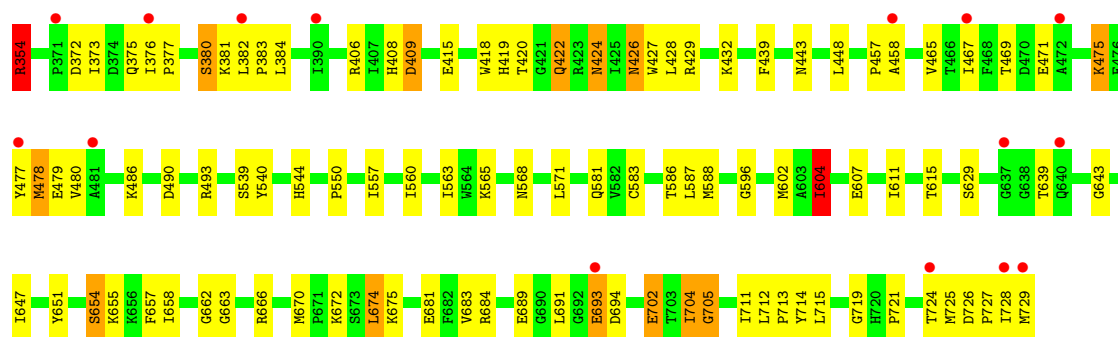
Chain D: 77% 21% •



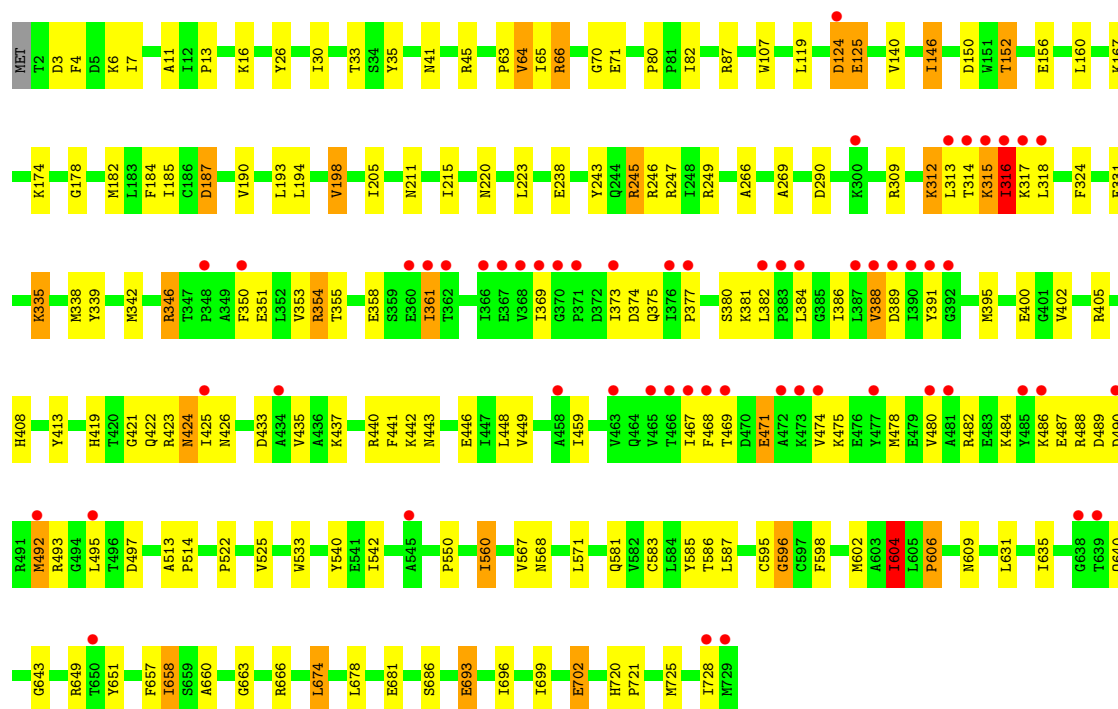
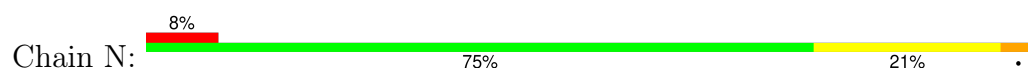
- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

Chain M: 3% 76% 20% • •

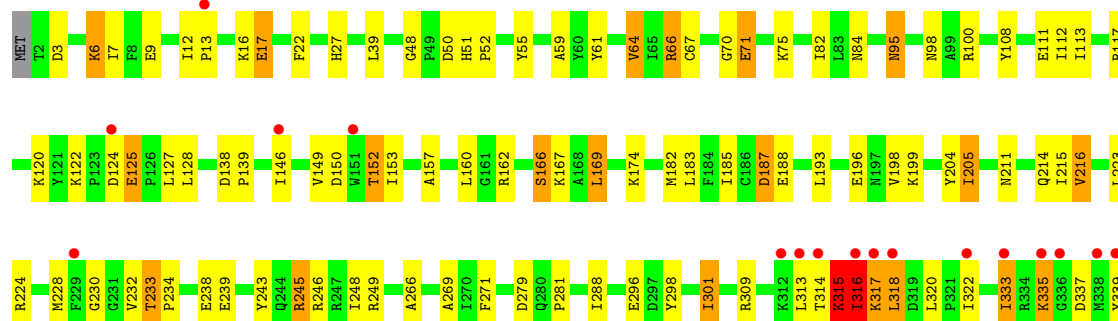




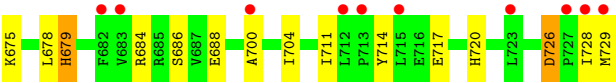
• Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



• 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, α , β , γ	99.65Å 136.87Å 140.86Å 101.26° 109.11° 104.08°	Depositor
Resolution (Å)	36.96 – 2.15 36.96 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.3 (36.96-2.15) 92.3 (36.96-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.242 0.187 , 0.240	Depositor DCC
R_{free} test set	16243 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	45096	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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: NI, SF4, ACT, GOL, NA, XCC, CU1

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	1.35	9/5244 (0.2%)	1.24	13/7106 (0.2%)
1	B	1.41	18/5231 (0.3%)	1.27	28/7086 (0.4%)
1	C	1.35	21/5193 (0.4%)	1.24	16/7038 (0.2%)
1	D	1.22	8/5212 (0.2%)	1.22	17/7062 (0.2%)
2	M	1.22	10/5921 (0.2%)	1.19	19/8015 (0.2%)
2	N	1.24	11/5928 (0.2%)	1.22	23/8023 (0.3%)
2	O	1.14	13/5883 (0.2%)	1.29	49/7965 (0.6%)
2	P	1.07	6/5885 (0.1%)	1.15	13/7968 (0.2%)
All	All	1.25	96/44497 (0.2%)	1.23	178/60263 (0.3%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	725	MET	C-O	-9.29	1.12	1.24
2	O	478	MET	CA-C	8.62	1.64	1.52
2	P	316	ILE	C-N	-7.73	1.23	1.33
1	C	415	ASN	C-O	-7.57	1.12	1.23
2	N	107	TRP	C-O	-7.50	1.15	1.24
1	C	415	ASN	N-CA	-7.39	1.35	1.46
1	C	417	PRO	C-O	-7.19	1.14	1.23
1	C	415	ASN	CA-C	-7.02	1.43	1.53
1	D	311	ASN	CA-C	6.96	1.61	1.53
1	B	89	ILE	CA-CB	6.91	1.64	1.54
1	B	578	ALA	CA-CB	-6.75	1.42	1.53
2	O	419	HIS	CG-ND1	-6.70	1.30	1.38
1	A	370	ARG	N-CA	-6.67	1.38	1.46
1	D	415	ASN	N-CA	-6.64	1.38	1.46
1	B	120	ILE	C-O	-6.63	1.16	1.24
2	N	475	LYS	N-CA	-6.63	1.37	1.46
1	C	291	ILE	CA-CB	6.56	1.62	1.54
1	D	346	ILE	CA-CB	6.48	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	153	ILE	CA-CB	6.45	1.60	1.53
1	C	246	HIS	C-O	-6.39	1.16	1.24
1	C	137	VAL	CA-CB	6.36	1.60	1.53
1	C	159	VAL	CA-CB	6.32	1.62	1.54
1	C	332	THR	CA-CB	6.31	1.62	1.53
1	B	236	ARG	CA-C	6.30	1.60	1.52
2	O	419	HIS	ND1-CE1	-6.22	1.26	1.32
2	P	212	PHE	C-O	-6.16	1.18	1.24
2	O	288	ILE	N-CA	6.14	1.50	1.45
1	B	537	ILE	CA-CB	6.12	1.60	1.53
2	M	264	ALA	CA-C	6.11	1.60	1.52
1	C	464	VAL	CA-CB	6.09	1.62	1.54
1	A	464	VAL	CA-CB	6.09	1.61	1.54
1	B	100	ARG	C-O	-6.09	1.17	1.24
1	C	635	GLU	N-CA	6.08	1.53	1.46
2	N	140	VAL	CA-CB	6.06	1.62	1.54
2	O	419	HIS	CD2-NE2	-6.06	1.31	1.37
1	B	19	VAL	C-O	-6.04	1.17	1.24
2	O	426	ASN	CA-C	-6.01	1.44	1.53
1	D	484	VAL	CA-CB	6.01	1.61	1.54
1	D	203	VAL	CA-CB	5.99	1.61	1.54
2	O	427	TRP	N-CA	-5.98	1.38	1.46
1	C	318	THR	CA-C	5.95	1.60	1.52
1	A	236	ARG	C-O	-5.93	1.17	1.24
1	B	429	ALA	CA-CB	5.92	1.61	1.53
1	B	631	TYR	C-O	-5.89	1.16	1.23
1	C	541	LEU	C-O	-5.86	1.16	1.24
1	C	203	VAL	N-CA	5.83	1.52	1.46
2	N	525	VAL	CA-CB	5.79	1.62	1.54
1	A	214	GLU	C-O	-5.79	1.17	1.24
2	N	65	ILE	CA-CB	-5.74	1.47	1.54
1	D	394	ILE	CA-CB	5.72	1.61	1.54
1	A	61	ILE	CA-CB	5.60	1.60	1.54
2	P	80	PRO	CA-C	5.54	1.57	1.52
2	N	87	ARG	CA-C	5.54	1.59	1.52
1	B	194	ARG	N-CA	5.53	1.53	1.46
2	M	467	ILE	CA-CB	5.48	1.60	1.53
1	D	318	THR	CA-C	5.47	1.59	1.52
2	M	639	THR	CA-C	5.47	1.59	1.52
1	C	283	HIS	N-CA	5.45	1.52	1.46
1	B	658	VAL	CA-CB	5.45	1.60	1.54
2	P	198	VAL	CA-CB	5.43	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	150	VAL	C-O	-5.42	1.17	1.24
2	N	190	VAL	CA-CB	5.41	1.60	1.54
2	O	683	VAL	CA-CB	5.38	1.61	1.54
2	M	221	TYR	C-O	-5.34	1.17	1.24
2	N	64	VAL	C-O	-5.34	1.18	1.24
2	N	595	CYS	CA-C	5.32	1.57	1.53
1	B	176	ARG	C-O	-5.32	1.17	1.23
1	D	352	ASP	CA-C	5.32	1.55	1.52
2	M	28	GLY	N-CA	5.27	1.52	1.45
2	O	687	VAL	CA-CB	5.26	1.60	1.54
1	A	89	ILE	N-CA	-5.26	1.40	1.46
2	M	465	VAL	CA-CB	5.26	1.62	1.54
2	O	685	ARG	C-N	5.26	1.40	1.33
1	C	313	VAL	C-O	-5.25	1.18	1.23
1	A	165	GLU	CA-C	5.21	1.59	1.52
1	C	17	PRO	C-O	5.21	1.29	1.23
2	P	73	VAL	C-O	5.18	1.29	1.24
2	O	685	ARG	CA-CB	-5.17	1.45	1.53
1	B	165	GLU	C-O	-5.16	1.18	1.24
1	C	420	ILE	CA-CB	5.16	1.59	1.53
1	A	420	ILE	CA-C	5.15	1.57	1.53
1	B	214	GLU	CA-C	5.11	1.59	1.52
1	A	194	ARG	N-CA	5.08	1.52	1.46
1	B	123	ALA	N-CA	-5.08	1.39	1.46
2	M	25	VAL	CA-CB	5.07	1.60	1.54
1	C	332	THR	C-O	5.07	1.28	1.24
1	C	334	PHE	CA-C	5.06	1.59	1.52
2	N	475	LYS	C-O	-5.05	1.17	1.24
1	C	524	LEU	CA-C	5.04	1.59	1.52
2	N	33	THR	CA-CB	5.03	1.61	1.53
2	M	629	SER	N-CA	5.02	1.52	1.46
2	P	650	THR	CA-CB	5.02	1.61	1.53
2	M	639	THR	CA-CB	5.02	1.61	1.53
1	B	238	ALA	CA-CB	5.01	1.61	1.53
2	M	604	ILE	CA-CB	5.01	1.59	1.54
1	B	203	VAL	CA-CB	5.00	1.61	1.54

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	480	VAL	N-CA-C	-12.86	99.04	110.74
2	O	476	GLU	N-CA-C	-11.60	98.64	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	479	GLU	N-CA-C	-10.78	99.23	112.38
2	O	473	LYS	N-CA-C	10.26	122.54	111.36
2	O	723	LEU	N-CA-C	9.77	121.53	111.07
2	O	474	VAL	N-CA-C	-9.57	99.09	111.05
1	A	344	GLY	N-CA-C	-9.21	103.24	115.21
2	O	471	GLU	N-CA-C	8.80	120.96	111.36
2	O	554	GLU	N-CA-C	8.55	122.84	109.07
1	A	574	VAL	N-CA-C	8.14	115.63	108.63
2	O	419	HIS	ND1-CE1-NE2	7.96	116.36	108.40
2	O	726	ASP	N-CA-C	7.88	122.21	110.39
2	N	728	ILE	N-CA-C	-7.79	103.32	111.58
2	O	344	GLY	N-CA-C	7.63	127.50	113.76
2	P	86	LYS	N-CA-C	7.55	119.59	111.36
2	O	477	TYR	N-CA-C	7.54	119.57	111.36
1	B	548	GLY	N-CA-C	7.46	119.09	111.56
1	B	317	CYS	N-CA-C	7.45	119.48	111.36
2	M	128	LEU	CA-C-N	-7.42	112.74	120.38
2	M	128	LEU	C-N-CA	-7.42	112.74	120.38
2	N	720	HIS	CA-C-N	7.39	127.10	119.56
2	N	720	HIS	C-N-CA	7.39	127.10	119.56
2	O	419	HIS	ND1-CG-CD2	7.25	113.35	106.10
2	O	478	MET	CA-C-N	7.18	132.10	120.60
2	O	478	MET	C-N-CA	7.18	132.10	120.60
2	N	513	ALA	CA-C-N	7.12	127.44	119.32
2	N	513	ALA	C-N-CA	7.12	127.44	119.32
1	B	120	ILE	N-CA-C	7.08	117.22	110.42
1	B	101	ASN	N-CA-C	7.08	118.78	111.14
2	P	316	ILE	N-CA-C	7.07	124.05	109.34
1	D	416	ARG	N-CA-C	7.02	125.33	109.81
2	O	685	ARG	N-CA-CB	-7.00	99.83	110.12
2	N	382	LEU	CA-C-N	-6.99	113.46	120.31
2	N	382	LEU	C-N-CA	-6.99	113.46	120.31
1	C	334	PHE	N-CA-C	6.87	119.40	111.02
1	B	318	THR	N-CA-C	-6.83	103.91	111.36
2	N	567	VAL	N-CA-C	-6.80	103.58	111.00
2	O	491	ARG	N-CA-C	-6.78	95.62	108.17
1	C	357	MET	CA-C-N	-6.69	112.70	120.12
1	C	357	MET	C-N-CA	-6.69	112.70	120.12
2	O	407	ILE	N-CA-C	-6.68	106.49	111.90
2	M	80	PRO	N-CA-C	6.67	118.84	110.70
2	O	490	ASP	N-CA-C	6.64	124.95	110.80
2	O	301	ILE	N-CA-C	6.64	116.79	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	361	ILE	N-CA-C	6.63	117.85	108.17
2	O	478	MET	N-CA-C	6.61	124.89	110.80
2	M	705	GLY	N-CA-C	6.60	120.25	110.42
2	O	427	TRP	N-CA-CB	-6.54	100.83	111.24
1	A	470	CYS	N-CA-C	6.52	119.34	109.63
1	D	580	ALA	CA-C-N	6.50	126.19	119.56
1	D	580	ALA	C-N-CA	6.50	126.19	119.56
1	C	411	ARG	N-CA-C	-6.48	104.14	111.14
2	N	604	ILE	CB-CA-C	-6.47	101.57	111.08
1	B	284	ASN	N-CA-C	6.46	118.22	109.24
2	O	342	MET	N-CA-C	6.42	118.82	109.07
2	P	268	GLY	N-CA-C	-6.37	104.31	113.86
2	O	546	GLY	CA-C-N	6.36	125.93	119.19
2	O	546	GLY	C-N-CA	6.36	125.93	119.19
2	O	233	THR	CB-CA-C	-6.31	99.26	109.67
2	M	384	LEU	N-CA-C	6.22	119.39	108.75
1	B	611	GLU	N-CA-C	6.17	118.80	111.71
2	O	573	THR	N-CA-C	6.16	119.26	111.69
2	M	316	ILE	N-CA-C	6.10	122.03	109.34
2	O	682	PHE	N-CA-C	6.08	117.99	111.36
1	A	283	HIS	N-CA-C	6.08	121.55	114.62
1	A	150	VAL	N-CA-C	6.08	117.32	111.91
1	D	495	VAL	N-CA-C	6.02	116.97	108.36
2	N	346	ARG	N-CA-C	-6.02	104.68	112.68
1	D	141	ALA	N-CA-C	-5.89	104.77	111.07
2	O	48	GLY	CA-C-N	5.89	125.57	119.56
2	O	48	GLY	C-N-CA	5.89	125.57	119.56
1	D	539	ILE	N-CA-C	5.88	121.56	109.34
2	M	689	GLU	N-CA-C	-5.87	106.16	113.38
1	B	357	MET	CA-C-N	-5.87	113.94	120.45
1	B	357	MET	C-N-CA	-5.87	113.94	120.45
1	C	283	HIS	N-CA-C	5.86	121.30	114.62
1	D	42	ASP	N-CA-C	5.82	117.30	111.07
2	P	128	LEU	CA-C-N	5.82	126.37	120.38
2	P	128	LEU	C-N-CA	5.82	126.37	120.38
2	N	314	THR	CB-CA-C	-5.80	98.87	110.42
2	O	128	LEU	CA-C-N	-5.79	114.42	120.38
2	O	128	LEU	C-N-CA	-5.79	114.42	120.38
2	O	725	MET	N-CA-C	-5.79	98.48	110.80
2	O	426	ASN	CB-CA-C	-5.77	99.51	113.19
1	D	519	TYR	N-CA-C	5.76	120.96	113.88
2	P	134	GLY	N-CA-C	-5.73	101.81	111.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	276	VAL	CA-C-N	-5.72	115.65	123.14
2	M	276	VAL	C-N-CA	-5.72	115.65	123.14
1	B	416	ARG	CA-C-N	-5.71	114.38	120.03
1	B	416	ARG	C-N-CA	-5.71	114.38	120.03
2	M	557	ILE	N-CA-C	-5.66	107.32	111.90
1	B	600	VAL	N-CA-CB	-5.65	103.30	111.21
1	A	81	THR	N-CA-C	-5.59	106.45	113.28
1	B	334	PHE	N-CA-C	5.58	117.83	111.02
2	M	691	LEU	N-CA-C	-5.57	106.84	113.97
1	B	470	CYS	N-CA-C	5.56	118.46	109.79
1	A	191	ASN	N-CA-C	5.55	117.23	110.41
2	O	84	ASN	N-CA-C	5.55	117.33	111.28
1	B	16	ALA	CA-C-N	-5.54	114.25	119.85
1	B	16	ALA	C-N-CA	-5.54	114.25	119.85
1	D	334	PHE	N-CA-C	5.50	117.73	111.02
2	O	468	PHE	N-CA-C	5.50	117.75	109.23
1	B	206	PHE	CA-C-N	5.46	125.82	121.61
1	B	206	PHE	C-N-CA	5.46	125.82	121.61
1	A	269	GLY	N-CA-C	-5.46	108.17	115.32
1	B	662	VAL	N-CA-C	5.46	115.66	110.42
1	D	159	VAL	N-CA-CB	5.45	118.75	110.58
2	N	318	LEU	CA-C-N	-5.43	115.11	122.77
2	N	318	LEU	C-N-CA	-5.43	115.11	122.77
1	B	471	ASN	N-CA-C	-5.42	101.74	110.14
2	M	354	ARG	N-CA-C	5.41	117.49	108.99
2	O	517	VAL	N-CA-C	5.41	115.84	107.78
1	B	600	VAL	CA-C-N	-5.39	114.37	119.76
1	B	600	VAL	C-N-CA	-5.39	114.37	119.76
1	C	539	ILE	N-CA-C	5.37	117.80	111.09
2	M	666	ARG	N-CA-C	5.35	119.06	112.54
2	O	301	ILE	CB-CA-C	-5.33	105.14	111.97
1	A	594	TRP	CA-CB-CG	5.33	123.73	113.60
2	O	12	ILE	CA-C-N	5.33	126.50	119.84
2	O	12	ILE	C-N-CA	5.33	126.50	119.84
1	C	492	ASN	N-CA-C	5.29	119.02	112.24
2	N	702	GLU	CB-CA-C	-5.29	99.16	110.32
1	D	173	ASP	N-CA-C	-5.26	106.37	112.89
1	C	432	SER	N-CA-C	-5.25	103.95	110.41
2	N	119	LEU	N-CA-C	-5.24	105.99	112.38
2	P	604	ILE	N-CA-C	5.23	116.33	109.58
1	A	120	ILE	N-CA-C	5.22	115.94	110.62
1	A	186	LEU	N-CA-C	-5.21	104.53	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	222	ALA	N-CA-C	5.21	119.97	111.37
2	P	19	VAL	N-CA-C	5.19	115.96	110.72
2	M	119	LEU	N-CA-C	-5.18	105.75	111.71
2	O	424	ASN	N-CA-C	5.18	116.93	111.28
2	N	41	ASN	N-CA-C	5.18	117.01	111.36
2	P	37	GLU	N-CA-C	5.17	116.60	111.07
2	P	720	HIS	CA-C-N	5.17	126.30	119.84
2	P	720	HIS	C-N-CA	5.17	126.30	119.84
2	O	449	VAL	N-CA-C	5.16	115.82	110.82
1	A	111	ALA	N-CA-C	5.15	116.90	111.28
1	C	175	ARG	N-CA-C	5.15	118.72	112.23
2	N	80	PRO	CA-C-N	-5.15	113.73	119.19
2	N	80	PRO	C-N-CA	-5.15	113.73	119.19
2	O	432	LYS	N-CA-C	-5.15	105.67	111.28
1	D	417	PRO	N-CA-C	-5.14	102.88	111.26
2	O	67	CYS	N-CA-C	5.13	116.56	110.97
1	A	321	GLU	N-CA-C	5.12	117.26	111.11
1	B	120	ILE	CA-C-O	-5.12	115.74	121.17
1	D	371	ILE	N-CA-C	-5.12	101.04	108.36
1	C	159	VAL	N-CA-CB	5.11	117.49	110.54
1	D	8	SER	CA-C-N	-5.11	116.19	122.84
1	D	8	SER	C-N-CA	-5.11	116.19	122.84
2	O	55	TYR	CA-C-N	-5.11	115.46	120.52
2	O	55	TYR	C-N-CA	-5.11	115.46	120.52
2	N	3	ASP	N-CA-C	5.10	119.79	111.37
2	N	80	PRO	N-CA-C	5.09	116.91	110.70
2	M	604	ILE	CB-CA-C	-5.09	103.60	111.08
1	D	284	ASN	N-CA-C	5.08	116.31	109.24
1	B	394	ILE	N-CA-C	5.08	115.70	110.36
1	B	646	LEU	CA-C-N	5.08	127.05	120.44
1	B	646	LEU	C-N-CA	5.08	127.05	120.44
1	C	591	ILE	N-CA-C	5.08	115.30	110.42
2	M	63	PRO	N-CA-C	5.08	120.22	113.57
2	N	649	ARG	N-CA-C	5.08	116.81	111.28
2	M	272	THR	CB-CA-C	-5.06	100.90	110.01
2	O	373	ILE	CB-CA-C	5.06	115.51	111.06
1	B	176	ARG	N-CA-C	5.05	117.55	110.23
2	P	166	SER	N-CA-C	5.05	116.79	111.28
1	C	204	VAL	CA-C-N	-5.05	114.75	119.85
1	C	204	VAL	C-N-CA	-5.05	114.75	119.85
1	C	268	MET	N-CA-C	5.04	118.53	112.38
2	N	316	ILE	N-CA-C	-5.04	98.85	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	662	GLY	N-CA-C	5.04	121.70	114.64
1	C	70	PHE	N-CA-C	5.04	119.06	113.01
2	O	425	ILE	N-CA-C	5.03	114.42	106.32
2	O	472	ALA	N-CA-C	5.03	117.72	111.24
1	C	113	HIS	N-CA-C	5.03	116.76	111.28
1	D	254	ILE	N-CA-C	5.02	115.24	110.42
2	P	149	VAL	N-CA-C	5.02	117.36	111.09
1	B	360	ILE	N-CA-CB	5.01	117.36	110.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5128	0	5128	68	0
1	B	5121	0	5134	75	0
1	C	5094	0	5097	93	0
1	D	5119	0	5115	112	0
2	M	5778	0	5736	104	0
2	N	5784	0	5749	108	0
2	O	5749	0	5716	394	0
2	P	5746	0	5710	151	0
3	A	16	0	0	0	0
3	B	8	0	0	1	0
3	C	16	0	0	1	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	1	0
3	O	8	0	0	2	0
3	P	8	0	0	0	0
4	A	9	0	0	1	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	2	0
5	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	7	0	0
5	C	6	0	8	5	0
5	D	6	0	8	6	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0
6	O	1	0	0	0	0
6	P	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	M	3	0	3	0	0
8	N	3	0	3	0	0
8	O	3	0	3	1	0
8	P	3	0	3	1	0
9	M	1	0	0	0	0
9	N	1	0	0	0	0
9	O	1	0	0	0	0
9	P	1	0	0	0	0
10	A	215	0	0	5	0
10	B	288	0	0	4	0
10	C	169	0	0	6	0
10	D	151	0	0	4	0
10	M	218	0	0	5	0
10	N	227	0	0	6	0
10	O	27	0	0	2	0
10	P	118	0	0	6	0
All	All	45096	0	43428	1063	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1063) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:482:ARG:HA	2:O:482:ARG:CZ	1.72	1.19
2:P:588:MET:HE1	2:P:604:ILE:HD13	1.17	1.17
2:O:490:ASP:HB2	2:O:491:ARG:NH1	1.61	1.16
2:O:685:ARG:O	2:O:688:GLU:HB3	1.44	1.15
2:O:482:ARG:HA	2:O:482:ARG:NH1	1.62	1.13
2:M:602:MET:HE3	2:M:647:ILE:HD13	1.31	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:335:LYS:HD2	2:M:335:LYS:H	1.07	1.12
2:O:477:TYR:O	2:O:480:VAL:HB	1.51	1.10
2:N:335:LYS:H	2:N:335:LYS:CD	1.66	1.09
2:N:335:LYS:HD3	2:N:335:LYS:N	1.65	1.08
2:O:490:ASP:HB2	2:O:491:ARG:HH12	1.09	1.08
2:M:602:MET:CE	2:M:647:ILE:HD13	1.84	1.08
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.19	1.07
2:P:588:MET:CE	2:P:604:ILE:HD13	1.88	1.04
2:O:420:THR:OG1	2:O:427:TRP:HE3	1.38	1.04
2:O:487:GLU:HG2	2:O:488:ARG:N	1.67	1.04
2:O:557:ILE:HD11	2:O:565:LYS:HG3	1.35	1.03
2:N:246[B]:ARG:HH12	2:N:247:ARG:NH1	1.56	1.02
2:O:427:TRP:C	2:O:428:LEU:HD22	1.85	1.02
2:P:444:TYR:O	2:P:448:LEU:HD22	1.60	1.02
2:O:371:PRO:HD2	2:O:469:THR:OG1	1.56	1.01
2:N:315:LYS:HE2	2:N:315:LYS:H	1.22	1.01
2:O:604:ILE:HD12	2:O:606:PRO:HD3	1.41	1.00
2:O:483:GLU:O	2:O:486:LYS:HB3	1.59	1.00
2:N:335:LYS:H	2:N:335:LYS:HD3	0.83	1.00
2:O:466:THR:C	2:O:467:ILE:HD12	1.86	0.99
2:O:351:GLU:HG2	2:O:423:ARG:H	1.27	0.99
2:O:723:LEU:HD23	2:O:723:LEU:C	1.86	0.99
2:O:483:GLU:CG	2:O:484:LYS:H	1.77	0.97
2:O:483:GLU:HG3	2:O:484:LYS:N	1.77	0.96
2:O:487:GLU:HG2	2:O:488:ARG:H	1.26	0.96
2:O:343:GLY:CA	2:O:349:ALA:HB2	1.95	0.96
2:O:348:PRO:CB	2:O:475:LYS:HE2	1.94	0.95
2:O:487:GLU:CG	2:O:488:ARG:N	2.30	0.95
2:O:348:PRO:HB3	2:O:475:LYS:HE2	1.48	0.95
2:O:482:ARG:CZ	2:O:482:ARG:CA	2.44	0.95
2:O:391:TYR:CD2	2:O:462:ARG:HB2	2.00	0.95
2:O:418:TRP:CH2	2:O:420:THR:HG21	2.02	0.94
2:O:348:PRO:CG	2:O:475:LYS:HE2	1.97	0.94
2:O:418:TRP:CH2	2:O:420:THR:CG2	2.51	0.93
1:D:539:ILE:HG23	1:D:540:GLY:N	1.84	0.92
2:N:484:LYS:HG2	10:N:1375:HOH:O	1.68	0.92
2:O:418:TRP:CZ3	2:O:420:THR:HG23	2.05	0.92
2:O:351:GLU:HB2	2:O:426:ASN:ND2	1.85	0.92
2:M:335:LYS:HD2	2:M:335:LYS:N	1.86	0.91
2:P:13:PRO:HB2	2:P:16:LYS:HG3	1.53	0.91
2:O:367:GLU:OE2	2:O:369:ILE:HD11	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:483:GLU:CG	2:O:484:LYS:N	2.30	0.90
2:P:602:MET:CE	2:P:647:ILE:HG21	2.02	0.90
2:O:370:GLY:HA3	2:O:469:THR:HG1	1.38	0.88
2:M:341:GLU:OE1	2:M:381:LYS:HE3	1.73	0.87
2:O:480:VAL:O	2:O:483:GLU:HG2	1.74	0.87
2:N:315:LYS:HE2	2:N:315:LYS:N	1.90	0.87
2:O:376:ILE:HG21	2:O:382:LEU:HD21	1.56	0.86
2:O:351:GLU:HB3	2:O:423:ARG:N	1.89	0.86
2:O:351:GLU:CG	2:O:423:ARG:H	1.88	0.86
1:D:416:ARG:O	1:D:418:VAL:HG23	1.76	0.86
2:M:335:LYS:H	2:M:335:LYS:CD	1.88	0.86
2:O:666:ARG:NH2	2:O:725:MET:HE2	1.90	0.85
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.05	0.85
2:O:715:LEU:HD22	2:O:720:HIS:HD2	1.40	0.85
2:P:470:ASP:HA	10:P:1362:HOH:O	1.75	0.85
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.56	0.85
2:O:653:VAL:O	2:O:685:ARG:HD2	1.77	0.84
2:O:370:GLY:HA3	2:O:469:THR:OG1	1.79	0.83
2:O:685:ARG:NH1	2:O:685:ARG:HB3	1.93	0.83
2:O:350:PHE:CD2	2:O:385:GLY:HA3	2.14	0.82
2:O:365:LYS:HG2	2:O:464:GLN:HG3	1.60	0.82
2:O:418:TRP:CZ3	2:O:420:THR:CG2	2.62	0.82
2:P:4:PHE:HB2	2:P:238:GLU:OE2	1.79	0.82
5:D:863:GOL:H2	2:P:27:HIS:HE1	1.43	0.82
2:O:723:LEU:HD23	2:O:723:LEU:O	1.79	0.82
2:O:396:GLN:HG3	2:O:399:PHE:CD1	2.15	0.81
2:P:150:ASP:OD2	2:P:152:THR:HG22	1.79	0.81
5:C:863:GOL:H31	2:O:27:HIS:CE1	2.15	0.81
2:O:419:HIS:HE1	2:O:421:GLY:O	1.64	0.80
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.61	0.80
2:M:704:ILE:HD11	2:M:711:ILE:HA	1.61	0.80
2:P:588:MET:HE1	2:P:604:ILE:CD1	2.06	0.80
1:C:577[A]:VAL:HG21	1:C:645:ILE:HG23	1.62	0.80
1:D:539:ILE:CG2	1:D:540:GLY:N	2.44	0.80
2:O:348:PRO:CG	2:O:475:LYS:CE	2.59	0.80
2:O:490:ASP:CB	2:O:491:ARG:NH1	2.42	0.80
2:O:350:PHE:HD2	2:O:385:GLY:HA3	1.42	0.80
2:O:351:GLU:CB	2:O:426:ASN:HD21	1.95	0.80
1:C:220:HIS:HD2	1:C:221:MET:O	1.65	0.79
2:O:343:GLY:HA2	2:O:349:ALA:HB2	1.65	0.79
2:O:421:GLY:HA3	2:O:425:ILE:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ALA:HB3	1:A:537:ILE:CD1	2.12	0.79
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.19	0.78
2:N:490:ASP:O	2:N:493:ARG:HG3	1.84	0.78
2:O:467:ILE:HD12	2:O:467:ILE:N	1.98	0.78
2:O:351:GLU:HG2	2:O:423:ARG:N	1.99	0.78
2:O:351:GLU:HB2	2:O:426:ASN:HD21	1.46	0.78
2:O:381:LYS:O	2:O:383:PRO:HD3	1.84	0.77
1:B:529:LYS:CB	10:B:1156:HOH:O	2.32	0.77
2:M:320:LEU:HB3	2:M:321:PRO:HD2	1.66	0.77
2:M:471:GLU:O	2:M:475:LYS:HB2	1.83	0.77
2:P:361:ILE:HG13	2:P:464:GLN:HG2	1.67	0.77
2:O:396:GLN:NE2	2:O:399:PHE:CD1	2.51	0.77
2:O:480:VAL:HA	2:O:483:GLU:OE1	1.84	0.77
5:C:863:GOL:H31	2:O:27:HIS:HE1	1.46	0.77
2:M:7:ILE:HD13	2:M:245:ARG:HD2	1.64	0.77
2:M:426:ASN:HD22	2:M:426:ASN:H	1.32	0.77
2:O:363:ASP:OD1	2:O:462:ARG:HA	1.85	0.77
1:B:529:LYS:HB3	10:B:1156:HOH:O	1.85	0.76
1:D:577[A]:VAL:HG21	1:D:645:ILE:HG23	1.67	0.76
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.21	0.76
2:N:346:ARG:HB3	2:N:381:LYS:HD2	1.66	0.76
2:O:649:ARG:HA	2:O:652:ILE:HD12	1.66	0.76
2:O:723:LEU:C	2:O:723:LEU:CD2	2.59	0.76
2:O:483:GLU:HG2	2:O:484:LYS:H	1.48	0.76
2:P:359:SER:C	2:P:361:ILE:H	1.93	0.76
1:C:614:ASP:H	5:C:863:GOL:H32	1.51	0.76
1:B:35:GLU:OE1	1:B:421:PRO:HB3	1.86	0.75
2:P:424:ASN:H	2:P:424:ASN:HD22	1.32	0.75
1:A:284:ASN:HD22	1:A:286:LEU:H	1.34	0.75
5:D:863:GOL:H2	2:P:27:HIS:CE1	2.21	0.75
2:N:478:MET:O	2:N:482:ARG:HG3	1.85	0.75
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.68	0.75
2:M:602:MET:HE3	2:M:647:ILE:CD1	2.15	0.75
2:P:150:ASP:OD2	2:P:152:THR:CG2	2.35	0.75
2:O:396:GLN:OE1	2:O:396:GLN:C	2.30	0.75
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.52	0.75
2:N:602:MET:HE1	2:N:658:ILE:HG21	1.68	0.74
2:O:476:GLU:C	2:O:476:GLU:OE1	2.30	0.74
2:O:478:MET:O	2:O:481:ALA:HB3	1.88	0.74
2:O:384:LEU:HD12	2:O:385:GLY:H	1.52	0.74
2:O:484:LYS:O	2:O:485:TYR:C	2.30	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:464:GLN:NE2	2:O:466:THR:HG23	2.02	0.73
1:C:209:HIS:HD2	1:D:213:SER:CB	2.02	0.73
1:C:60:LYS:O	1:C:64:GLU:HG3	1.87	0.73
2:O:371:PRO:CD	2:O:469:THR:OG1	2.34	0.73
2:O:351:GLU:O	2:O:352:LEU:HB3	1.88	0.73
2:O:374:ASP:HB3	2:O:440:ARG:NE	2.03	0.73
2:P:316:ILE:HG23	2:P:316:ILE:O	1.88	0.73
1:A:577[B]:VAL:HG11	1:A:645:ILE:HG23	1.69	0.72
2:M:406:ARG:NH1	2:M:409:ASP:OD2	2.20	0.72
1:A:192:GLU:O	1:A:196:GLU:HG3	1.88	0.72
2:O:480:VAL:HG12	2:O:481:ALA:N	2.02	0.72
2:O:353:VAL:HG12	2:O:388:VAL:HB	1.72	0.72
1:D:510:LEU:HD12	1:D:510:LEU:N	2.05	0.72
2:O:491:ARG:NH1	2:O:491:ARG:H	1.88	0.71
2:O:349:ALA:HB3	2:O:424:ASN:O	1.91	0.71
2:O:351:GLU:HB3	2:O:423:ARG:CA	2.20	0.71
2:O:347:THR:HG23	2:O:383:PRO:HG3	1.72	0.71
2:O:626:MET:HB2	2:O:631:LEU:HD13	1.73	0.71
2:O:355:THR:OG1	2:O:395:MET:HG3	1.91	0.70
2:O:650:THR:HG22	2:O:650:THR:O	1.91	0.70
2:O:157:ALA:HB3	2:O:183:LEU:HD22	1.71	0.70
2:O:349:ALA:HB1	2:O:426:ASN:OD1	1.91	0.70
2:O:557:ILE:CD1	2:O:565:LYS:HG3	2.17	0.70
2:O:666:ARG:NH2	2:O:725:MET:CE	2.54	0.70
2:P:505:SER:HB3	2:P:570:TYR:CE2	2.26	0.70
2:P:670:MET:HE3	2:P:675:LYS:HG2	1.74	0.70
2:O:384:LEU:C	2:O:474:VAL:HG21	2.17	0.70
2:O:343:GLY:HA3	2:O:349:ALA:HB2	1.72	0.70
2:O:396:GLN:HG3	2:O:399:PHE:HD1	1.56	0.70
1:D:299:GLU:OE2	1:D:299:GLU:HA	1.91	0.69
2:O:509:CYS:HB3	8:O:953:ACT:H3	1.74	0.69
2:O:666:ARG:CZ	2:O:725:MET:CE	2.71	0.69
2:O:478:MET:O	2:O:481:ALA:N	2.25	0.69
2:O:124:ASP:C	2:O:125:GLU:HG2	2.18	0.69
2:O:480:VAL:O	2:O:481:ALA:C	2.34	0.69
2:N:384:LEU:HD11	2:N:467:ILE:CG2	2.22	0.69
2:O:396:GLN:HE22	2:O:398:ASP:HB2	1.57	0.69
2:O:374:ASP:HB3	2:O:440:ARG:HE	1.58	0.69
2:O:427:TRP:O	2:O:428:LEU:HD22	1.93	0.69
2:O:728:ILE:O	2:O:728:ILE:HD12	1.92	0.68
2:O:473:LYS:C	2:O:476:GLU:H	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:615:LEU:C	1:C:615:LEU:HD23	2.18	0.68
2:O:108:TYR:O	2:O:112:ILE:HG13	1.93	0.68
2:O:524:ARG:O	2:O:524:ARG:HG3	1.93	0.68
2:M:588:MET:HE1	2:M:604:ILE:HG23	1.76	0.68
1:C:601:PRO:HD3	1:C:652:ARG:NH2	2.09	0.68
2:O:685:ARG:O	2:O:688:GLU:CB	2.33	0.68
2:P:486:LYS:HA	2:P:489:ASP:HB2	1.76	0.67
2:P:602:MET:HE3	2:P:647:ILE:HG21	1.76	0.67
2:O:333:ILE:HD12	2:O:429:ARG:HB3	1.76	0.67
2:P:149:VAL:HG11	8:P:953:ACT:H3	1.76	0.67
2:N:408:HIS:HD2	2:N:419:HIS:ND1	1.91	0.67
2:O:486:LYS:O	2:O:489:ASP:HB3	1.93	0.67
1:D:614:ASP:N	5:D:863:GOL:H11	2.09	0.67
2:M:439:PHE:CE1	2:M:443:ASN:HB2	2.29	0.67
2:O:162:ARG:HG3	2:O:188:GLU:HB2	1.77	0.67
2:M:377:PRO:O	2:M:380:SER:HB3	1.94	0.67
2:O:348:PRO:HG2	2:O:475:LYS:CE	2.25	0.67
2:O:605:LEU:HB3	2:O:608:CYS:HB2	1.77	0.67
1:A:655:LYS:NZ	1:A:674:TYR:O	2.28	0.67
1:D:68:CYS:HB2	1:D:97:ILE:CG2	2.24	0.67
2:O:360:GLU:O	2:O:361:ILE:HB	1.94	0.67
2:O:365:LYS:HG2	2:O:464:GLN:CG	2.24	0.66
2:M:23:ARG:NH1	10:M:793:HOH:O	2.27	0.66
2:P:80:PRO:HB2	2:P:81:PRO:HD3	1.76	0.66
1:C:209:HIS:HD2	1:D:213:SER:OG	1.78	0.66
2:M:424:ASN:HD22	2:M:424:ASN:H	1.43	0.66
2:P:444:TYR:O	2:P:448:LEU:CD2	2.39	0.66
2:O:691:LEU:HD21	2:O:721:PRO:HG2	1.76	0.66
2:O:340:VAL:HG21	2:O:382:LEU:HB2	1.78	0.66
2:O:351:GLU:CB	2:O:426:ASN:ND2	2.56	0.66
2:P:341:GLU:CD	2:P:427:TRP:HE1	2.04	0.66
1:C:213:SER:CB	1:D:209:HIS:HD2	2.08	0.65
1:D:149[A]:ARG:HD3	10:D:1162:HOH:O	1.96	0.65
1:D:284:ASN:HD22	1:D:286:LEU:H	1.42	0.65
2:M:426:ASN:HD22	2:M:426:ASN:N	1.94	0.65
2:O:230:GLY:HA3	2:O:243:TYR:CE2	2.32	0.65
2:O:670:MET:HE2	2:O:674:LEU:HG	1.77	0.65
2:O:342:MET:O	2:O:427:TRP:HA	1.95	0.65
2:O:469:THR:O	2:O:470:ASP:HB2	1.95	0.65
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.09	0.65
2:M:602:MET:HE1	2:M:657:PHE:HE2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:224:ARG:O	2:O:228:MET:HB2	1.95	0.65
2:O:715:LEU:HD22	2:O:720:HIS:CD2	2.29	0.65
2:O:3:ASP:O	2:O:6:LYS:HG2	1.97	0.65
2:O:422:GLN:N	2:O:422:GLN:OE1	2.30	0.65
2:O:384:LEU:HD13	2:O:468:PHE:O	1.97	0.65
2:O:685:ARG:HB3	2:O:685:ARG:HH11	1.62	0.65
1:C:98:VAL:O	1:C:102:VAL:HG12	1.97	0.64
1:C:260:GLN:HG2	10:C:1398:HOH:O	1.97	0.64
2:O:407:ILE:HG23	2:O:411:ILE:HD13	1.77	0.64
2:O:428:LEU:HD22	2:O:428:LEU:N	2.12	0.64
2:M:655:LYS:HE3	10:M:901:HOH:O	1.96	0.64
2:O:469:THR:O	2:O:470:ASP:CB	2.45	0.64
1:D:515:ASN:HA	1:D:518:THR:HG22	1.80	0.64
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.32	0.64
1:D:195:LYS:O	1:D:199:ARG:HG3	1.97	0.64
2:N:335:LYS:CD	2:N:335:LYS:N	2.40	0.64
1:C:587:LYS:O	1:C:591:ILE:HG13	1.98	0.64
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.28	0.64
2:N:246[B]:ARG:HH12	2:N:247:ARG:HH11	1.43	0.64
2:N:443:ASN:ND2	2:N:446:GLU:OE1	2.30	0.64
2:M:314:THR:O	2:M:315:LYS:C	2.39	0.64
2:M:721:PRO:O	2:M:725:MET:HG3	1.97	0.64
2:O:352:LEU:CD1	2:O:484:LYS:HG3	2.28	0.63
2:O:508:LEU:HD23	3:O:900:SF4:S1	2.38	0.63
2:N:150:ASP:OD2	2:N:152:THR:HG22	1.99	0.63
2:O:482:ARG:CA	2:O:482:ARG:NE	2.59	0.63
2:M:344:GLY:O	2:M:346:ARG:NH1	2.32	0.63
2:O:447:ILE:O	2:O:451:LYS:HB2	1.98	0.63
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.34	0.63
2:N:492:MET:HG2	10:N:1002:HOH:O	1.97	0.63
2:N:540:TYR:CD1	2:N:550:PRO:HD3	2.34	0.63
2:N:609:ASN:ND2	2:N:666:ARG:HH12	1.97	0.62
2:O:169:LEU:HD13	2:O:193:LEU:CD2	2.29	0.62
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.34	0.62
1:C:294:ALA:O	1:C:298:MET:HG2	1.99	0.62
1:C:587:LYS:H	1:D:220:HIS:HE1	1.48	0.62
2:M:568:ASN:HD21	2:M:581:GLN:HE21	1.48	0.62
1:C:615:LEU:HD23	1:C:615:LEU:O	2.00	0.62
2:N:315:LYS:N	2:N:315:LYS:CE	2.63	0.62
2:O:64:VAL:HB	2:O:223:LEU:HD12	1.81	0.62
1:C:23:LYS:HE3	10:C:931:HOH:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:404:GLU:OE1	2:O:423:ARG:NE	2.34	0.61
2:O:564:TRP:HB2	2:O:567:VAL:HB	1.82	0.61
2:P:666:ARG:HD2	2:P:728:ILE:HD12	1.81	0.61
2:N:316:ILE:O	2:N:317:LYS:C	2.42	0.61
2:N:354:ARG:HD2	2:N:389:ASP:OD2	2.00	0.61
1:B:200:THR:OG1	1:B:201:HIS:HD2	1.84	0.61
2:O:490:ASP:O	2:O:492:MET:N	2.33	0.61
2:P:583:CYS:CB	2:P:586:THR:HG22	2.30	0.61
1:A:114:CYS:HB2	10:A:1315:HOH:O	2.00	0.61
2:O:95:ASN:ND2	2:O:98:ASN:H	1.98	0.61
2:M:348:PRO:HD2	2:M:383:PRO:HB3	1.82	0.61
2:P:66:ARG:O	2:P:70:GLY:HA2	2.01	0.61
2:P:316:ILE:O	2:P:316:ILE:CG2	2.49	0.61
1:C:220:HIS:HE1	1:D:587:LYS:H	1.49	0.61
2:M:704:ILE:HD13	2:M:714:TYR:CB	2.30	0.61
2:O:385:GLY:N	2:O:474:VAL:HG21	2.16	0.61
2:O:420:THR:O	2:O:426:ASN:HA	2.00	0.61
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.81	0.61
2:P:289:PRO:O	2:P:290:ASP:HB2	2.00	0.61
1:A:122:HIS:HD2	10:A:902:HOH:O	1.83	0.61
2:O:478:MET:O	2:O:482:ARG:N	2.33	0.61
2:P:166:SER:HB2	2:P:196:GLU:OE2	1.99	0.61
2:P:359:SER:O	2:P:361:ILE:N	2.34	0.61
2:M:342:MET:SD	2:M:342:MET:N	2.73	0.61
2:O:360:GLU:O	2:O:361:ILE:CB	2.49	0.61
2:O:351:GLU:CB	2:O:423:ARG:N	2.62	0.60
1:B:515:ASN:HA	1:B:518:THR:HG23	1.84	0.60
2:O:420:THR:HG1	2:O:427:TRP:HE3	0.65	0.60
2:M:457:PRO:O	2:M:458:ALA:HB3	2.00	0.60
2:O:346:ARG:HH22	2:O:381:LYS:NZ	2.00	0.60
2:P:726:ASP:OD1	2:P:726:ASP:N	2.33	0.60
2:O:557:ILE:HD11	2:O:565:LYS:CG	2.22	0.60
2:P:602:MET:HG3	2:P:647:ILE:HD13	1.83	0.60
1:A:220:HIS:HD2	1:A:221:MET:O	1.84	0.60
2:O:351:GLU:CB	2:O:423:ARG:H	2.15	0.60
1:D:399:THR:O	1:D:403:MET:HG3	2.02	0.60
2:O:388:VAL:HG13	2:O:465:VAL:HG22	1.84	0.60
2:P:428:LEU:N	2:P:428:LEU:HD12	2.16	0.60
2:O:426:ASN:OD1	2:O:426:ASN:N	2.34	0.59
2:P:199:LYS:HE2	2:P:415:GLU:OE2	2.03	0.59
2:N:560:ILE:O	2:N:660:ALA:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:167:LYS:HD3	2:M:196:GLU:OE1	2.01	0.59
2:O:347:THR:CG2	2:O:383:PRO:HG3	2.32	0.59
2:O:712:LEU:HB3	2:O:713:PRO:CD	2.31	0.59
1:D:510:LEU:HD12	1:D:510:LEU:H	1.65	0.59
1:A:535:ALA:HB3	1:A:537:ILE:HD12	1.85	0.59
2:P:238:GLU:HG2	10:P:735:HOH:O	2.01	0.59
2:O:169:LEU:HD13	2:O:193:LEU:HD21	1.85	0.59
1:A:284:ASN:HD21	1:A:286:LEU:HG	1.68	0.59
1:D:149[A]:ARG:NH2	1:D:250:ASP:OD2	2.36	0.59
2:P:340:VAL:HG21	2:P:376:ILE:HD11	1.85	0.59
2:N:384:LEU:HD11	2:N:467:ILE:HG23	1.85	0.58
2:O:467:ILE:N	2:O:467:ILE:CD1	2.65	0.58
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.34	0.58
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.85	0.58
2:O:470:ASP:O	2:O:474:VAL:HG12	2.02	0.58
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.68	0.58
2:P:488:ARG:C	2:P:490:ASP:H	2.12	0.58
1:A:316:CYS:H	1:A:503:GLN:HE22	1.52	0.58
1:C:112:ALA:HA	1:D:217:ASN:HD22	1.69	0.58
2:N:150:ASP:OD2	2:N:152:THR:CG2	2.52	0.58
1:B:615:LEU:HD23	1:B:615:LEU:C	2.29	0.58
2:P:457:PRO:O	2:P:458:ALA:HB2	2.03	0.58
1:C:456:ILE:HD13	1:C:463:GLY:HA2	1.86	0.58
2:O:95:ASN:C	2:O:95:ASN:HD22	2.11	0.58
1:B:661[A]:GLU:HG3	1:B:665:ARG:HH21	1.66	0.58
2:O:367:GLU:OE1	2:O:369:ILE:HG12	2.04	0.58
2:O:665:ALA:O	2:O:722:ALA:HB2	2.03	0.58
1:A:220:HIS:HE1	1:B:587:LYS:H	1.52	0.57
1:D:466:LEU:HD22	1:D:595:TRP:HZ2	1.66	0.57
2:O:355:THR:HG21	2:O:395:MET:HB3	1.86	0.57
2:O:396:GLN:OE1	2:O:397:ALA:N	2.37	0.57
1:A:177:LEU:HB2	1:A:180:GLU:CD	2.29	0.57
1:C:577[B]:VAL:HG23	1:C:649:LEU:CD2	2.35	0.57
1:D:577[A]:VAL:HG21	1:D:645:ILE:CG2	2.34	0.57
2:P:318:LEU:HD13	2:P:320:LEU:HD11	1.85	0.57
1:C:368:HIS:HE1	1:C:416:ARG:CB	2.18	0.57
2:O:384:LEU:CD1	2:O:468:PHE:O	2.53	0.57
2:O:478:MET:C	2:O:480:VAL:N	2.62	0.57
2:O:613:ILE:HD12	2:O:670:MET:HE3	1.85	0.57
2:O:464:GLN:HE22	2:O:466:THR:HG23	1.67	0.57
2:O:6:LYS:O	2:O:9:GLU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:568:ASN:ND2	2:P:581:GLN:HB2	2.19	0.57
2:N:315:LYS:CE	2:N:315:LYS:CA	2.78	0.57
2:M:602:MET:HE1	2:M:647:ILE:HD13	1.80	0.57
2:O:685:ARG:HB3	2:O:685:ARG:CZ	2.31	0.57
2:P:359:SER:C	2:P:361:ILE:N	2.61	0.57
1:C:138:LYS:HG3	1:C:255:LEU:O	2.05	0.57
2:P:602:MET:HE3	2:P:647:ILE:CG2	2.34	0.57
1:B:267:ASN:O	1:B:270:VAL:HG22	2.05	0.56
2:M:727:PRO:HG3	2:O:367:GLU:HG2	1.86	0.56
2:O:477:TYR:O	2:O:480:VAL:CB	2.41	0.56
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.87	0.56
1:A:399:THR:HG22	1:A:403:MET:HE3	1.86	0.56
1:D:128:ALA:HA	1:D:160:LEU:HD22	1.87	0.56
2:O:157:ALA:HB3	2:O:183:LEU:HD23	1.87	0.56
1:B:368:HIS:NE2	1:B:416:ARG:HD2	2.20	0.56
2:O:232:VAL:CG1	2:O:239:GLU:HB3	2.35	0.56
2:O:623:PRO:HA	2:O:707:THR:HA	1.86	0.56
1:C:357:MET:O	1:C:360:ILE:HG12	2.05	0.56
1:D:469:GLY:C	4:D:800:XCC:S1	2.88	0.56
2:O:340:VAL:HG23	2:O:382:LEU:H	1.70	0.56
1:B:577[A]:VAL:HG21	1:B:645:ILE:HG23	1.88	0.56
2:P:150:ASP:CG	2:P:152:THR:HG22	2.30	0.56
2:N:246[B]:ARG:NH1	2:N:247:ARG:NH1	2.41	0.56
2:N:369:ILE:HD12	2:N:468:PHE:CE2	2.41	0.56
2:O:483:GLU:HG3	2:O:484:LYS:H	1.44	0.56
1:A:335:ALA:H	1:A:471:ASN:HD22	1.52	0.56
1:B:2:PRO:N	1:B:625:SER:HG	2.03	0.56
2:O:248:ILE:O	2:O:309:ARG:NH2	2.37	0.56
1:A:126:GLU:OE1	1:A:390:THR:OG1	2.21	0.55
2:O:649:ARG:HA	2:O:652:ILE:CD1	2.34	0.55
1:D:149[B]:ARG:NH2	1:D:250:ASP:OD2	2.38	0.55
2:N:315:LYS:HE2	2:N:315:LYS:CA	2.36	0.55
1:C:213:SER:OG	1:D:209:HIS:HD2	1.89	0.55
1:D:220:HIS:HD2	1:D:221:MET:O	1.88	0.55
2:M:354:ARG:HH21	2:M:480:VAL:HG11	1.71	0.55
2:M:408:HIS:HD2	2:M:419:HIS:ND1	2.05	0.55
2:N:342:MET:SD	2:N:342:MET:N	2.79	0.55
2:O:666:ARG:CZ	2:O:725:MET:HE2	2.37	0.55
2:O:685:ARG:C	2:O:688:GLU:HB3	2.27	0.55
2:O:333:ILE:HD12	2:O:429:ARG:CB	2.36	0.55
2:O:473:LYS:O	2:O:476:GLU:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:602:MET:HE1	2:O:645:MET:HE2	1.89	0.55
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.88	0.55
1:C:217:ASN:HD22	1:D:112:ALA:HA	1.71	0.55
2:N:482:ARG:O	2:N:486[A]:LYS:HG3	2.05	0.55
2:O:398:ASP:C	2:O:400:GLU:H	2.15	0.55
1:D:144:LYS:O	1:D:148:ARG:HG3	2.06	0.55
2:O:340:VAL:CG2	2:O:382:LEU:H	2.19	0.55
2:O:430:VAL:HG12	2:O:431:SER:N	2.21	0.55
2:P:424:ASN:H	2:P:424:ASN:ND2	2.01	0.55
2:O:396:GLN:CG	2:O:399:PHE:CD1	2.90	0.55
2:P:602:MET:CE	2:P:645:MET:HE3	2.38	0.54
1:C:614:ASP:H	5:C:863:GOL:C3	2.18	0.54
2:N:442:LYS:HB2	10:N:1326:HOH:O	2.06	0.54
1:C:68:CYS:HB2	1:C:97:ILE:HG23	1.90	0.54
2:N:721:PRO:O	2:N:725:MET:HG3	2.07	0.54
2:O:721:PRO:O	2:O:725:MET:HB2	2.07	0.54
2:P:424:ASN:HD22	2:P:424:ASN:N	1.99	0.54
1:B:539:ILE:HG13	1:B:540:GLY:H	1.72	0.54
1:A:213:SER:OG	1:B:209:HIS:HD2	1.90	0.54
1:B:35:GLU:OE2	1:B:423:ILE:HD11	2.07	0.54
2:M:602:MET:HE1	2:M:657:PHE:CE2	2.43	0.54
2:P:522:PRO:HD3	2:P:533:TRP:CD1	2.43	0.54
2:M:117[B]:ARG:CZ	2:M:127:LEU:HD23	2.37	0.54
2:O:720:HIS:ND1	2:O:721:PRO:HD2	2.22	0.54
1:C:129:GLU:OE2	1:C:164:GLN:NE2	2.40	0.54
2:O:500:VAL:HG22	2:O:502:THR:H	1.73	0.54
2:P:383:PRO:HB2	2:P:474:VAL:HG21	1.90	0.54
1:C:182:GLU:HG2	1:C:204:VAL:HG11	1.88	0.54
2:O:342:MET:SD	2:O:428:LEU:HB2	2.48	0.54
2:O:396:GLN:CG	2:O:399:PHE:HD1	2.21	0.54
2:O:481:ALA:O	2:O:482:ARG:C	2.51	0.54
2:M:490:ASP:HA	2:M:493:ARG:NH1	2.23	0.53
2:O:421:GLY:C	2:O:422:GLN:OE1	2.50	0.53
1:B:28:THR:HG21	1:B:33:VAL:HG12	1.91	0.53
1:C:408:PHE:O	1:C:411:ARG:HB3	2.07	0.53
1:D:313:VAL:HG21	1:D:331:VAL:HG13	1.90	0.53
2:O:396:GLN:C	2:O:396:GLN:CD	2.76	0.53
1:B:201:HIS:HE1	2:N:35:TYR:OH	1.91	0.53
1:B:444:ASN:HB3	1:B:451:VAL:HG23	1.91	0.53
1:B:529:LYS:HB2	10:B:1156:HOH:O	2.01	0.53
1:C:214:GLU:O	1:C:217:ASN:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:565:LYS:O	2:O:569:ASP:CG	2.51	0.53
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.74	0.53
2:O:351:GLU:HB3	2:O:426:ASN:HD21	1.70	0.53
1:A:201:HIS:CE1	2:M:35:TYR:OH	2.61	0.53
1:B:656:LEU:HD22	1:B:660:LYS:HD2	1.89	0.53
2:O:478:MET:O	2:O:481:ALA:CB	2.54	0.53
1:D:614:ASP:H	5:D:863:GOL:H11	1.72	0.53
2:N:400:GLU:HB3	2:N:488:ARG:NH2	2.24	0.53
2:O:424:ASN:ND2	2:O:485:TYR:CE1	2.76	0.53
1:B:220:HIS:HD2	1:B:221:MET:O	1.92	0.52
1:C:577[B]:VAL:HG23	1:C:649:LEU:HD23	1.90	0.52
2:O:483:GLU:O	2:O:486:LYS:CB	2.47	0.52
2:P:408:HIS:HD2	2:P:419:HIS:ND1	2.07	0.52
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.39	0.52
1:D:587:LYS:HE3	4:D:800:XCC:S4	2.49	0.52
2:N:587:LEU:HD22	2:N:602:MET:HE2	1.91	0.52
1:A:209:HIS:HD2	1:B:213:SER:OG	1.92	0.52
2:N:350:PHE:CD1	2:N:350:PHE:C	2.87	0.52
2:O:351:GLU:HB3	2:O:423:ARG:HA	1.91	0.52
2:O:424:ASN:CG	2:O:485:TYR:HE1	2.16	0.52
2:O:666:ARG:CZ	2:O:725:MET:HE1	2.40	0.52
1:A:535:ALA:CB	1:A:537:ILE:CD1	2.87	0.52
2:O:316:ILE:HG13	2:O:454:GLU:HG3	1.92	0.52
2:O:612:MET:HB3	2:O:669:TRP:HB3	1.90	0.52
2:P:583:CYS:HB2	2:P:586:THR:HG22	1.92	0.52
1:C:655:LYS:NZ	1:C:674:TYR:O	2.33	0.52
2:O:602:MET:CE	2:O:645:MET:HE2	2.40	0.52
2:M:478:MET:O	2:M:478:MET:HG3	2.09	0.52
2:N:583:CYS:HB2	2:N:586:THR:HG22	1.90	0.52
1:D:24:ASN:O	1:D:27:ARG:HG2	2.08	0.52
2:O:488:ARG:HG3	2:O:488:ARG:NH1	2.24	0.52
2:M:272:THR:HG22	2:M:272:THR:O	2.10	0.52
2:O:367:GLU:OE2	2:O:369:ILE:CD1	2.53	0.52
2:O:467:ILE:HG22	2:O:468:PHE:N	2.25	0.52
2:P:369:ILE:HD13	2:P:473:LYS:HD2	1.92	0.52
2:P:505:SER:HB3	2:P:570:TYR:HE2	1.74	0.52
1:D:238:ALA:O	1:D:241:ASP:HB3	2.10	0.51
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.91	0.51
2:O:367:GLU:HB3	2:O:466:THR:HG22	1.91	0.51
2:O:506:CYS:HB3	3:O:900:SF4:S4	2.51	0.51
2:P:583:CYS:SG	2:P:589:GLU:HG2	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:426:ASN:H	2:M:426:ASN:ND2	2.05	0.51
2:N:187:ASP:HA	2:N:211:ASN:ND2	2.23	0.51
2:O:698:LYS:HG2	2:O:718:LYS:HD2	1.92	0.51
2:P:583:CYS:HB3	2:P:586:THR:HG22	1.92	0.51
1:C:221:MET:HE2	1:D:584:MET:HE2	1.91	0.51
1:D:18:ARG:NE	1:D:636:MET:HE3	2.25	0.51
2:M:351:GLU:OE2	2:M:422:GLN:HA	2.11	0.51
2:O:66:ARG:NH1	2:O:234:PRO:HG2	2.25	0.51
2:O:478:MET:C	2:O:480:VAL:H	2.18	0.51
2:P:425:ILE:HG22	2:P:425:ILE:O	2.10	0.51
1:B:153:GLU:OE1	1:B:155:GLU:CD	2.54	0.51
1:D:364:ALA:HB1	1:D:369:THR:HB	1.92	0.51
2:O:166:SER:HB2	2:O:196:GLU:CG	2.41	0.51
2:O:626:MET:SD	2:O:631:LEU:HD12	2.51	0.51
2:O:684:ARG:NH1	2:O:685:ARG:HG2	2.25	0.51
2:P:422:GLN:HE21	2:P:422:GLN:N	2.08	0.51
2:P:585:TYR:CE2	2:P:656:LYS:HD2	2.45	0.51
1:C:281:HIS:HB3	1:C:351:VAL:HG12	1.92	0.51
2:N:266:ALA:O	2:N:269:ALA:HB3	2.09	0.51
1:D:118:ASN:C	1:D:118:ASN:HD22	2.19	0.51
1:D:284:ASN:ND2	1:D:286:LEU:H	2.08	0.51
2:N:596:GLY:HA2	2:N:598:PHE:CE2	2.45	0.51
2:O:113:ILE:O	2:O:117:ARG:HG3	2.10	0.51
2:O:473:LYS:O	2:O:476:GLU:CB	2.58	0.51
2:P:684:ARG:O	2:P:688:GLU:HG3	2.11	0.51
1:C:209:HIS:CD2	1:D:213:SER:CB	2.89	0.51
2:M:372:ASP:H	2:M:375:GLN:NE2	2.09	0.51
2:O:384:LEU:HD12	2:O:385:GLY:N	2.25	0.51
2:O:482:ARG:CZ	2:O:482:ARG:N	2.74	0.51
2:O:484:LYS:O	2:O:485:TYR:O	2.29	0.51
2:O:490:ASP:CB	2:O:491:ARG:HH11	2.24	0.51
2:P:358:GLU:HG3	2:P:391:TYR:CE2	2.46	0.51
2:O:160:LEU:HD13	2:O:215:ILE:HD13	1.93	0.50
2:O:365:LYS:CG	2:O:464:GLN:HG3	2.35	0.50
2:O:435:VAL:C	2:O:437:LYS:H	2.19	0.50
1:A:584:MET:HE3	1:B:73:ALA:CB	2.40	0.50
2:N:7:ILE:HD13	2:N:245:ARG:HD2	1.94	0.50
2:N:419:HIS:HE1	2:N:421:GLY:O	1.94	0.50
1:A:284:ASN:ND2	1:A:286:LEU:HG	2.26	0.50
2:O:403:LEU:O	2:O:452:MET:HE1	2.11	0.50
2:O:473:LYS:HA	2:O:476:GLU:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577[A]:VAL:HG13	1:C:649:LEU:HD23	1.92	0.50
2:O:346:ARG:HH22	2:O:381:LYS:HZ2	1.60	0.50
2:O:489:ASP:OD1	2:O:489:ASP:O	2.30	0.50
1:B:569:VAL:HA	1:B:672:GLN:HE22	1.77	0.50
2:M:587:LEU:HD23	2:M:588:MET:CE	2.42	0.50
2:N:13:PRO:HB2	2:N:16:LYS:HG3	1.93	0.50
2:O:66:ARG:O	2:O:70:GLY:HA2	2.12	0.50
2:O:316:ILE:CG1	2:O:454:GLU:HG3	2.41	0.50
2:O:417:LEU:HD22	2:O:444:TYR:HE1	1.76	0.50
2:P:266:ALA:O	2:P:269:ALA:HB3	2.11	0.50
2:M:67:CYS:HB2	2:M:227:MET:HE2	1.93	0.50
2:P:516:HIS:HE1	2:P:593:THR:O	1.94	0.50
1:C:577[A]:VAL:HG13	1:C:649:LEU:CD2	2.41	0.50
1:D:662:VAL:HG21	2:P:194:LEU:HD13	1.93	0.50
2:N:243:TYR:CZ	2:N:247:ARG:HD3	2.46	0.50
2:O:17:GLU:OE1	2:O:22:PHE:HE2	1.95	0.50
2:M:219:ALA:O	2:M:223:LEU:HG	2.12	0.50
2:N:568:ASN:ND2	2:N:581:GLN:HE21	2.09	0.50
2:O:481:ALA:O	2:O:485:TYR:HB2	2.12	0.50
2:N:124:ASP:OD1	2:N:125:GLU:OE1	2.30	0.49
2:O:344:GLY:O	2:O:345:ASN:OD1	2.30	0.49
2:O:420:THR:OG1	2:O:427:TRP:CE3	2.30	0.49
1:C:201:HIS:HE1	1:C:627:VAL:HG13	1.77	0.49
1:C:220:HIS:CD2	1:C:221:MET:O	2.55	0.49
1:D:260:GLN:NE2	10:D:1320:HOH:O	2.43	0.49
2:O:373:ILE:HG12	2:O:435:VAL:HG21	1.94	0.49
2:O:470:ASP:O	2:O:474:VAL:CG1	2.60	0.49
2:P:4:PHE:CB	2:P:238:GLU:OE2	2.57	0.49
1:C:114:CYS:HB2	10:C:1242:HOH:O	2.11	0.49
2:N:471:GLU:O	2:N:471:GLU:HG3	2.10	0.49
2:P:657:PHE:CE1	2:P:667:ILE:HD11	2.47	0.49
1:A:333:SER:CB	1:A:503:GLN:HE21	2.25	0.49
2:O:491:ARG:NH1	2:O:491:ARG:N	2.58	0.49
1:D:35:GLU:OE2	1:D:423:ILE:CD1	2.60	0.49
2:M:540:TYR:CD1	2:M:550:PRO:HD3	2.47	0.49
2:O:534:LEU:HD13	10:O:1263:HOH:O	2.13	0.49
1:C:69:ARG:HG2	1:C:75:PRO:HB3	1.94	0.49
1:D:559:LEU:O	1:D:563:MET:HG3	2.12	0.49
2:P:64:VAL:HG13	2:P:111:GLU:OE2	2.12	0.49
2:M:169:LEU:HD13	2:M:193:LEU:CD2	2.42	0.49
2:M:602:MET:CE	2:M:647:ILE:CD1	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:160:LEU:HD13	2:N:215:ILE:HD13	1.94	0.49
2:P:389:ASP:HB2	2:P:464:GLN:HG3	1.94	0.49
1:A:284:ASN:ND2	1:A:286:LEU:H	2.04	0.49
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.31	0.49
2:O:476:GLU:OE1	2:O:476:GLU:O	2.30	0.49
2:M:427:TRP:C	2:M:428:LEU:HD12	2.38	0.49
2:N:486[B]:LYS:HG3	2:N:487:GLU:N	2.27	0.49
2:N:489:ASP:O	2:N:493:ARG:HG2	2.13	0.49
2:O:59:ALA:HB2	2:O:630:THR:HA	1.94	0.49
1:D:201:HIS:HE1	2:P:35:TYR:OH	1.96	0.49
2:N:316:ILE:O	2:N:316:ILE:HG23	2.13	0.49
1:B:107:LEU:HD21	1:B:215:LEU:HB3	1.94	0.48
1:C:614:ASP:N	5:C:863:GOL:H32	2.24	0.48
1:B:291:ILE:HD13	1:B:397:ALA:HB1	1.95	0.48
1:D:215:LEU:HD22	1:D:234:ALA:HA	1.95	0.48
2:N:468:PHE:HB2	2:N:474:VAL:HG22	1.95	0.48
2:N:522:PRO:HD3	2:N:533:TRP:CD1	2.49	0.48
2:O:344:GLY:H	2:O:349:ALA:HB2	1.78	0.48
2:O:503:PHE:CZ	2:O:521:THR:HG22	2.48	0.48
2:P:341:GLU:HG3	2:P:429:ARG:HG2	1.95	0.48
2:N:63:PRO:HB2	2:N:220:ASN:HB2	1.95	0.48
2:O:354:ARG:O	2:O:390:ILE:N	2.42	0.48
2:O:468:PHE:CZ	2:O:477:TYR:OH	2.59	0.48
2:O:724:THR:C	2:O:725:MET:O	2.50	0.48
1:D:658:VAL:O	1:D:662:VAL:HG23	2.13	0.48
2:N:424:ASN:H	2:N:424:ASN:HD22	1.61	0.48
2:O:393:ARG:NH1	2:O:394:LYS:HG2	2.29	0.48
2:O:418:TRP:HH2	2:O:420:THR:HG21	1.68	0.48
2:P:150:ASP:OD2	2:P:152:THR:HG23	2.14	0.48
2:P:343:GLY:HA2	2:P:347:THR:O	2.13	0.48
2:M:320:LEU:HB3	2:M:321:PRO:CD	2.40	0.48
2:N:391:TYR:C	2:N:391:TYR:CD2	2.91	0.48
2:O:669:TRP:HA	2:O:700:ALA:O	2.13	0.48
1:B:201:HIS:CE1	2:N:35:TYR:OH	2.67	0.48
1:B:288:SER:O	1:B:292:VAL:HG23	2.12	0.48
1:B:606:THR:C	1:B:636:MET:HE2	2.39	0.48
1:D:515:ASN:HA	1:D:518:THR:CG2	2.42	0.48
1:D:539:ILE:CG2	1:D:540:GLY:H	2.27	0.48
2:M:604:ILE:HG13	2:M:643:GLY:O	2.14	0.48
2:N:497:ASP:OD2	2:N:585:TYR:OH	2.24	0.48
2:O:428:LEU:N	2:O:428:LEU:CD2	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG22	1:A:474:LYS:HG2	1.96	0.48
1:B:368:HIS:CD2	1:B:416:ARG:HD2	2.48	0.48
1:D:267:ASN:O	1:D:270:VAL:HG22	2.13	0.48
2:P:505:SER:CB	2:P:570:TYR:CE2	2.95	0.48
1:C:316:CYS:H	1:C:503:GLN:HE22	1.62	0.48
2:O:348:PRO:HG3	2:O:475:LYS:CE	2.43	0.48
2:O:487:GLU:O	2:O:490:ASP:CG	2.57	0.48
2:P:338:MET:SD	2:P:341:GLU:HB2	2.54	0.48
2:M:670:MET:HE3	2:M:675:LYS:HG3	1.96	0.48
2:N:609:ASN:ND2	2:N:666:ARG:NH1	2.61	0.48
2:O:430:VAL:CG1	2:O:434:ALA:HB3	2.43	0.48
2:O:657:PHE:O	2:O:658:ILE:C	2.57	0.48
1:C:615:LEU:C	1:C:615:LEU:CD2	2.85	0.47
1:D:28:THR:OG1	1:D:477:GLN:NE2	2.44	0.47
1:D:282:GLY:HA3	1:D:352:ASP:OD1	2.14	0.47
2:M:64:VAL:HA	2:M:223:LEU:HD12	1.96	0.47
2:N:4:PHE:N	2:N:238[B]:GLU:OE1	2.43	0.47
2:N:312:LYS:NZ	2:N:312:LYS:HB3	2.29	0.47
2:O:344:GLY:N	2:O:349:ALA:HB2	2.29	0.47
2:O:348:PRO:HG3	2:O:475:LYS:HE2	1.90	0.47
2:O:371:PRO:HD2	2:O:469:THR:CB	2.41	0.47
2:P:226:GLY:HA3	10:P:1355:HOH:O	2.13	0.47
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.45	0.47
2:O:490:ASP:O	2:O:493:ARG:N	2.42	0.47
2:O:491:ARG:CZ	2:O:491:ARG:HB2	2.43	0.47
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.28	0.47
1:B:661[A]:GLU:HG3	1:B:665:ARG:NH2	2.30	0.47
2:M:615:THR:HG21	2:M:674:LEU:HG	1.96	0.47
2:O:376:ILE:CG2	2:O:382:LEU:HD21	2.37	0.47
2:O:382:LEU:O	2:O:383:PRO:C	2.57	0.47
1:B:486:LYS:HE2	1:B:519:TYR:CE2	2.49	0.47
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.44	0.47
2:O:523:GLU:HB3	2:O:654:SER:OG	2.15	0.47
2:P:351:GLU:CG	2:P:426:ASN:HD21	2.27	0.47
1:C:635:GLU:C	1:C:636:MET:HE3	2.40	0.47
2:N:167:LYS:HG2	10:N:1288:HOH:O	2.14	0.47
2:O:351:GLU:HB3	2:O:423:ARG:H	1.70	0.47
2:O:477:TYR:O	2:O:478:MET:C	2.58	0.47
2:O:604:ILE:HA	2:O:611:ILE:HG22	1.95	0.47
2:O:653:VAL:O	2:O:685:ARG:CD	2.56	0.47
1:D:201:HIS:CE1	2:P:35:TYR:OH	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:609:ASN:HD21	2:N:666:ARG:HH12	1.60	0.47
2:O:279:ASP:C	2:O:279:ASP:OD1	2.57	0.47
2:O:352:LEU:HD11	2:O:484:LYS:HG3	1.95	0.47
2:O:480:VAL:O	2:O:481:ALA:O	2.32	0.47
1:B:298:MET:HE1	1:B:402:ARG:HG2	1.95	0.47
1:C:59:CYS:HB3	1:D:75:PRO:HG2	1.96	0.47
2:O:342:MET:HG3	2:O:384:LEU:HD23	1.97	0.47
2:O:431:SER:HB3	2:O:434:ALA:HB2	1.97	0.47
2:O:594:SER:O	2:O:636:GLY:HA2	2.14	0.47
1:A:201:HIS:HE1	2:M:35:TYR:OH	1.98	0.47
1:C:331:VAL:HG13	1:C:332:THR:N	2.30	0.47
1:D:510:LEU:N	1:D:510:LEU:CD1	2.77	0.47
2:O:138:ASP:N	2:O:139:PRO:CD	2.78	0.47
2:P:373:ILE:HD12	2:P:441:PHE:CE2	2.50	0.47
2:P:402:VAL:HG21	2:P:538:ALA:HB2	1.94	0.47
1:A:209:HIS:HD2	1:B:213:SER:CB	2.28	0.47
1:A:357:MET:O	1:A:360:ILE:HG12	2.14	0.47
2:O:510:GLN:NE2	2:O:516:HIS:O	2.39	0.47
2:O:650:THR:O	2:O:650:THR:CG2	2.60	0.47
1:C:293:GLN:HG2	10:C:1184:HOH:O	2.14	0.47
2:M:540:TYR:O	2:M:544:HIS:HD2	1.97	0.47
2:P:124:ASP:OD1	2:P:125:GLU:OE1	2.33	0.47
2:P:341:GLU:HG2	2:P:428:LEU:O	2.14	0.47
2:P:346:ARG:HH11	2:P:346:ARG:HB2	1.80	0.47
2:M:670:MET:SD	2:M:674:LEU:HD13	2.55	0.46
2:O:477:TYR:O	2:O:480:VAL:N	2.41	0.46
2:O:622:THR:OG1	2:O:626:MET:O	2.26	0.46
1:B:182:GLU:HG2	1:B:204:VAL:HG11	1.97	0.46
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.45	0.46
1:D:28:THR:HG21	1:D:33:VAL:CG1	2.44	0.46
2:N:178:GLY:HA3	2:N:317:LYS:HE2	1.97	0.46
1:B:114:CYS:SG	1:B:209:HIS:NE2	2.89	0.46
1:C:62:GLY:HA3	3:C:700:SF4:S4	2.55	0.46
2:O:95:ASN:ND2	2:O:95:ASN:C	2.74	0.46
2:P:275:PRO:CD	2:P:309:ARG:HD3	2.45	0.46
1:D:313:VAL:HG21	1:D:331:VAL:CG1	2.46	0.46
2:O:150:ASP:OD2	2:O:152:THR:HG23	2.14	0.46
2:O:590:ASN:N	2:O:591:PRO:HD3	2.30	0.46
2:P:602:MET:HE3	2:P:645:MET:HE3	1.97	0.46
2:N:64:VAL:HA	2:N:223:LEU:HD12	1.96	0.46
2:O:612:MET:SD	2:O:622:THR:HB	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:482:ARG:HA	2:P:485:TYR:CD1	2.50	0.46
2:P:700:ALA:HA	2:P:704:ILE:HD13	1.98	0.46
1:D:317:CYS:O	1:D:321:GLU:HG2	2.14	0.46
1:D:330:LEU:HD23	10:D:946:HOH:O	2.15	0.46
1:D:415:ASN:OD1	1:D:417:PRO:HD3	2.16	0.46
1:D:594:TRP:CE3	1:D:598:LEU:HD12	2.51	0.46
2:O:13:PRO:HB2	2:O:16:LYS:HB2	1.97	0.46
2:O:61:TYR:HD1	2:O:66:ARG:HD2	1.81	0.46
1:D:432:SER:HA	1:D:555:ARG:HD3	1.98	0.46
1:D:617:TYR:O	1:D:621:THR:OG1	2.32	0.46
1:D:636:MET:HE2	10:D:810:HOH:O	2.15	0.46
2:N:351:GLU:OE2	2:N:422:GLN:HA	2.16	0.46
2:N:568:ASN:HD21	2:N:581:GLN:HE21	1.64	0.46
2:O:271:PHE:CD2	2:O:271:PHE:C	2.94	0.46
1:B:466:LEU:HD22	1:B:595:TRP:CZ2	2.51	0.46
2:M:342:MET:HB3	2:M:382:LEU:O	2.16	0.46
2:M:457:PRO:O	2:M:458:ALA:CB	2.64	0.46
2:M:704:ILE:HG13	2:M:705:GLY:N	2.30	0.46
2:O:266:ALA:O	2:O:269:ALA:HB3	2.15	0.46
2:O:430:VAL:CG1	2:O:431:SER:N	2.79	0.46
1:A:61:ILE:HD13	1:A:77:ARG:HD2	1.97	0.46
1:A:584:MET:HG3	1:B:73:ALA:HB2	1.97	0.46
1:C:217:ASN:ND2	1:D:112:ALA:HA	2.31	0.46
2:M:344:GLY:O	2:M:345:ASN:HB2	2.16	0.46
2:O:199:LYS:HD2	2:O:204:TYR:OH	2.16	0.46
2:O:343:GLY:HA2	2:O:349:ALA:CB	2.42	0.46
2:O:427:TRP:NE1	2:O:429:ARG:NH2	2.64	0.46
2:P:138:ASP:N	2:P:139:PRO:CD	2.79	0.46
1:B:118:ASN:C	1:B:118:ASN:HD22	2.23	0.46
1:B:305:ALA:HB1	1:B:409:LYS:HE3	1.97	0.46
1:D:138:LYS:HG3	1:D:255:LEU:O	2.16	0.46
2:M:728:ILE:O	2:M:729:MET:HB2	2.15	0.46
2:O:337:ASP:O	2:O:432:LYS:N	2.49	0.46
2:O:385:GLY:N	2:O:474:VAL:CG2	2.78	0.46
2:O:471:GLU:O	2:O:475:LYS:HB2	2.15	0.46
2:O:374:ASP:HB3	2:O:440:ARG:CZ	2.46	0.45
2:P:313:LEU:HD13	2:P:315:LYS:HB2	1.99	0.45
2:P:588:MET:HE3	2:P:728:ILE:HG12	1.98	0.45
1:C:383:ALA:O	2:P:87:ARG:HD3	2.16	0.45
2:O:318:LEU:HD12	2:O:320:LEU:HD21	1.97	0.45
2:O:360:GLU:O	2:O:361:ILE:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:516:HIS:HD2	2:O:593:THR:OG1	1.98	0.45
2:O:653:VAL:C	2:O:685:ARG:HD2	2.39	0.45
2:P:61:TYR:HD1	2:P:66:ARG:HD2	1.81	0.45
2:P:124:ASP:OD2	2:P:124:ASP:N	2.41	0.45
2:P:420:THR:HG23	2:P:427:TRP:HB3	1.98	0.45
2:P:457:PRO:O	2:P:458:ALA:CB	2.64	0.45
1:A:126:GLU:HG2	1:A:131:LYS:HB2	1.97	0.45
1:A:299:GLU:O	1:A:303:LYS:HG3	2.15	0.45
2:M:333:ILE:HD12	2:M:418:TRP:HB2	1.98	0.45
2:M:477:TYR:C	2:M:479:GLU:H	2.25	0.45
2:O:474:VAL:HG13	2:O:475:LYS:N	2.30	0.45
2:O:670:MET:O	2:O:701:ASP:HB3	2.16	0.45
2:P:420:THR:CG2	2:P:427:TRP:HB3	2.46	0.45
2:M:587:LEU:HB3	2:M:588:MET:HE2	1.98	0.45
2:N:353:VAL:HG22	2:N:388:VAL:HB	1.98	0.45
2:O:7:ILE:HD13	2:O:245:ARG:HD2	1.99	0.45
1:B:25:ARG:O	1:B:49:PHE:HB3	2.17	0.45
1:C:615:LEU:O	1:C:619:ILE:HG13	2.16	0.45
1:D:496:VAL:HA	1:D:545:PHE:O	2.17	0.45
2:N:433:ASP:OD1	2:N:437:LYS:HE2	2.16	0.45
2:O:100:ARG:HB3	2:O:271:PHE:HB2	1.97	0.45
2:O:727:PRO:O	2:O:729:MET:N	2.50	0.45
1:A:125:VAL:O	1:A:129:GLU:HG3	2.17	0.45
1:C:384:TYR:HE2	2:P:88:ALA:CB	2.29	0.45
2:O:50:ASP:HA	2:O:75:LYS:HD2	1.99	0.45
2:O:232:VAL:HG11	2:O:239:GLU:HB3	1.97	0.45
2:O:396:GLN:CD	2:O:399:PHE:HD1	2.25	0.45
2:O:585:TYR:CZ	2:O:656:LYS:HD2	2.52	0.45
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.52	0.45
2:M:246:ARG:HE	2:M:247:ARG:NH1	2.14	0.45
2:O:350:PHE:O	2:O:385:GLY:HA2	2.16	0.45
2:O:391:TYR:CE2	2:O:462:ARG:HD2	2.52	0.45
1:A:113:HIS:HD1	1:A:241:ASP:CG	2.23	0.45
1:A:281:HIS:ND1	1:A:282:GLY:N	2.65	0.45
1:A:515:ASN:ND2	1:A:518:THR:HG21	2.32	0.45
2:M:657:PHE:O	2:M:663:GLY:HA2	2.17	0.45
2:N:66:ARG:O	2:N:70:GLY:HA2	2.17	0.45
2:N:384:LEU:CD1	2:N:467:ILE:CG2	2.93	0.45
1:C:238:ALA:O	1:C:241:ASP:HB3	2.17	0.45
1:C:468:CYS:HB2	10:C:693:HOH:O	2.17	0.45
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:417:LEU:HD21	2:P:439:PHE:CE1	2.52	0.45
1:D:515:ASN:OD1	1:D:518:THR:HG21	2.17	0.44
2:M:420:THR:HG22	2:M:427:TRP:HB3	1.97	0.44
2:N:247:ARG:NH2	2:N:514:PRO:HG3	2.32	0.44
2:P:361:ILE:HA	2:P:464:GLN:OE1	2.16	0.44
1:B:406:GLU:O	1:B:410:GLU:HG3	2.17	0.44
1:C:283:HIS:CD2	1:C:317:CYS:CB	2.98	0.44
1:D:261:PRO:HG3	1:D:431:TRP:CZ3	2.53	0.44
2:M:604:ILE:HA	2:M:611:ILE:HG22	1.99	0.44
2:N:342:MET:HG2	2:N:384:LEU:HB2	1.98	0.44
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.46	0.44
2:O:146:ILE:O	2:O:146:ILE:HG13	2.17	0.44
2:O:370:GLY:CA	2:O:469:THR:OG1	2.58	0.44
1:A:201:HIS:HE1	1:A:627:VAL:HG13	1.82	0.44
2:P:357:SER:O	2:P:361:ILE:HG22	2.17	0.44
2:P:426:ASN:O	2:P:427:TRP:HB2	2.16	0.44
1:B:515:ASN:CA	1:B:518:THR:HG23	2.47	0.44
2:M:317:LYS:HE2	10:M:862:HOH:O	2.18	0.44
2:M:712:LEU:HB3	2:M:713:PRO:HD3	1.98	0.44
2:O:657:PHE:CE1	2:O:667:ILE:HD11	2.52	0.44
1:B:238:ALA:O	1:B:241:ASP:HB3	2.18	0.44
2:M:651:TYR:O	2:M:654:SER:HB3	2.18	0.44
2:O:519:ILE:CG2	2:O:584:LEU:HD21	2.48	0.44
1:C:201:HIS:CE1	1:C:627:VAL:HG13	2.53	0.44
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.82	0.44
2:P:117[B]:ARG:HG2	2:P:127:LEU:HD13	2.00	0.44
1:D:284:ASN:HD22	1:D:284:ASN:C	2.26	0.44
1:D:455:ALA:HB1	1:D:460:GLU:HG3	1.98	0.44
2:P:318:LEU:HD13	2:P:320:LEU:CD1	2.47	0.44
1:C:126[A]:GLU:HG2	1:C:131:LYS:HB2	1.98	0.44
1:C:149:ARG:HG2	1:C:149:ARG:HH11	1.83	0.44
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.53	0.44
2:M:560:ILE:O	10:M:1386:HOH:O	2.21	0.44
2:N:490:ASP:HA	2:N:493:ARG:HD2	2.00	0.44
2:O:727:PRO:O	2:O:728:ILE:C	2.61	0.44
1:B:186:LEU:HD22	1:B:205:PRO:HD2	2.00	0.44
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.48	0.44
2:M:236:ALA:O	2:M:240:GLN:HG2	2.18	0.44
2:O:396:GLN:OE1	2:O:398:ASP:N	2.49	0.44
2:P:385:GLY:O	2:P:467:ILE:HA	2.17	0.44
2:P:589:GLU:O	2:P:590:ASN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:O	1:A:42:ASP:HB2	2.17	0.43
2:M:602:MET:HE2	2:M:602:MET:HB3	1.95	0.43
2:N:45:ARG:HD2	10:N:1293:HOH:O	2.18	0.43
2:O:584:LEU:HD23	2:O:592:MET:HE1	1.99	0.43
1:C:213:SER:CB	1:D:209:HIS:CD2	2.97	0.43
1:D:331:VAL:HG23	1:D:332:THR:H	1.82	0.43
1:D:358:PRO:HA	1:D:380:ILE:HD13	2.00	0.43
1:D:450:ARG:O	1:D:450:ARG:HG3	2.18	0.43
2:N:11:ALA:O	2:N:13:PRO:HD3	2.18	0.43
2:N:26:TYR:CE2	2:N:30:ILE:HD11	2.52	0.43
2:N:355:THR:HG23	2:N:395:MET:HG2	2.00	0.43
2:O:169:LEU:HD13	2:O:193:LEU:HG	2.01	0.43
2:O:473:LYS:O	2:O:476:GLU:N	2.45	0.43
1:A:657:GLY:O	1:A:661[A]:GLU:HG3	2.18	0.43
2:N:184:PHE:C	2:N:185:ILE:HG13	2.42	0.43
2:O:232:VAL:HG13	2:O:239:GLU:HB3	1.99	0.43
2:O:315:LYS:O	2:O:316:ILE:HB	2.18	0.43
2:O:462:ARG:O	2:O:463:VAL:HG23	2.19	0.43
2:P:358:GLU:O	2:P:462:ARG:NH2	2.51	0.43
2:P:576:ASN:O	2:P:577:ARG:HB2	2.18	0.43
2:P:678:LEU:O	2:P:679:HIS:C	2.61	0.43
2:P:711:ILE:O	2:P:714:TYR:HB3	2.18	0.43
1:A:492:ASN:HA	1:A:524:LEU:HB2	2.00	0.43
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.99	0.43
1:D:107:LEU:HD21	1:D:215:LEU:HB3	2.00	0.43
1:D:351:VAL:HB	1:D:356:ILE:HD13	2.01	0.43
2:M:3:ASP:O	2:M:6[A]:LYS:HB3	2.18	0.43
2:O:444:TYR:O	2:O:448:LEU:HD22	2.18	0.43
2:N:193:LEU:O	2:N:198:VAL:HG13	2.18	0.43
2:N:324:PHE:HA	2:N:413:TYR:O	2.19	0.43
1:A:297:GLU:OE1	1:A:398:LYS:NZ	2.42	0.43
1:D:453:ASN:ND2	1:D:566:ASP:HB3	2.34	0.43
2:M:583:CYS:HB3	2:M:586:THR:HG22	2.00	0.43
2:N:604:ILE:HB	2:N:606:PRO:HD3	2.01	0.43
2:P:504:TYR:CE2	2:P:550:PRO:HB3	2.54	0.43
1:A:186:LEU:HD22	1:A:205:PRO:HD2	2.01	0.43
1:B:414:SER:O	1:B:415:ASN:HB2	2.18	0.43
1:B:661[A]:GLU:CG	1:B:665:ARG:HH21	2.32	0.43
1:C:401:ILE:O	1:C:405:ILE:HG13	2.18	0.43
2:M:244:GLN:HG3	2:M:272:THR:CG2	2.48	0.43
2:N:560:ILE:N	2:N:560:ILE:HD13	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:HIS:HA	2:O:52:PRO:HD3	1.86	0.43
2:O:373:ILE:HG22	2:O:440:ARG:HG3	1.99	0.43
2:O:490:ASP:C	2:O:492:MET:N	2.76	0.43
2:O:584:LEU:O	2:O:585:TYR:HD2	2.01	0.43
2:P:361:ILE:HG21	2:P:391:TYR:HB2	2.00	0.43
1:B:65:GLY:O	1:B:97:ILE:HG22	2.19	0.43
1:C:557:VAL:CG2	1:C:594:TRP:CZ3	3.02	0.43
2:N:309:ARG:HA	2:N:309:ARG:HD2	1.87	0.43
2:N:604:ILE:H	2:N:604:ILE:HG13	1.57	0.43
2:O:423:ARG:HG2	2:O:423:ARG:HH11	1.84	0.43
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.95	0.43
2:M:335:LYS:HG3	2:M:429:ARG:HH12	1.84	0.43
2:N:441:PHE:CE1	2:N:469:THR:HG21	2.54	0.43
2:O:396:GLN:HG3	2:O:399:PHE:CE1	2.54	0.43
2:P:3:ASP:O	2:P:6:LYS:HB3	2.19	0.43
1:A:537:ILE:HG22	1:A:540:GLY:H	1.84	0.43
1:B:220:HIS:CD2	1:B:221:MET:O	2.71	0.43
1:B:308:LYS:HE3	1:B:308:LYS:HA	2.00	0.43
1:C:164:GLN:O	1:C:168:GLU:HG3	2.18	0.43
1:D:28:THR:HG21	1:D:33:VAL:HG12	2.00	0.43
1:D:126:GLU:OE1	1:D:390:THR:OG1	2.33	0.43
1:D:416:ARG:O	1:D:417:PRO:C	2.60	0.43
2:O:169:LEU:HD13	2:O:193:LEU:CG	2.49	0.43
2:P:79:LEU:HD22	2:P:112:ILE:HG12	2.01	0.43
1:A:12:ARG:NH2	10:A:1449:HOH:O	2.52	0.42
1:A:626:ASP:HB3	2:M:212:PHE:CG	2.54	0.42
1:C:622:GLN:O	1:C:625:SER:OG	2.30	0.42
1:D:20:MET:O	1:D:21:GLU:C	2.62	0.42
2:O:390:ILE:HG22	2:O:391:TYR:H	1.84	0.42
2:O:488:ARG:C	2:O:490:ASP:N	2.77	0.42
2:P:602:MET:HE1	2:P:645:MET:HE3	2.01	0.42
1:C:122:HIS:HD2	10:C:869:HOH:O	2.01	0.42
1:C:431:TRP:O	1:C:547:MET:HG2	2.19	0.42
1:D:142:LYS:O	1:D:143:LEU:C	2.59	0.42
1:D:339:LEU:O	1:D:340:ALA:C	2.62	0.42
2:N:657:PHE:O	2:N:663:GLY:HA2	2.17	0.42
2:O:587:LEU:HD13	2:O:602:MET:HE3	2.01	0.42
2:P:356:VAL:HG21	2:P:389:ASP:HB3	2.00	0.42
1:A:220:HIS:CD2	1:A:221:MET:O	2.70	0.42
1:C:216:VAL:HG12	1:D:108:THR:HA	2.00	0.42
2:M:588:MET:HE3	2:M:728:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:478:MET:O	2:O:481:ALA:CA	2.67	0.42
2:P:657:PHE:O	2:P:663:GLY:HA2	2.19	0.42
1:A:432:SER:HA	1:A:555:ARG:HD3	2.01	0.42
1:B:88:GLY:HA3	3:B:750:SF4:S3	2.60	0.42
1:B:515:ASN:HA	1:B:518:THR:CG2	2.47	0.42
1:A:30:ASP:OD2	1:A:507:LYS:NZ	2.45	0.42
1:C:196:GLU:OE2	2:O:120:LYS:HE3	2.20	0.42
1:D:18:ARG:CD	1:D:636:MET:HE3	2.49	0.42
2:N:354:ARG:HH21	2:N:480:VAL:HG11	1.83	0.42
2:O:459:ILE:HD11	2:O:542:ILE:HG21	1.99	0.42
2:O:482:ARG:HB3	2:O:483:GLU:H	1.67	0.42
2:O:488:ARG:CG	2:O:488:ARG:HH11	2.32	0.42
2:O:527:LEU:CD2	2:O:594:SER:HA	2.49	0.42
2:P:372:ASP:OD1	2:P:373:ILE:N	2.42	0.42
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.84	0.42
1:A:622:GLN:O	1:A:625:SER:OG	2.32	0.42
1:D:201:HIS:CE1	1:D:627:VAL:HG13	2.55	0.42
2:M:247:ARG:NH1	10:M:971:HOH:O	2.52	0.42
2:O:493:ARG:HH11	2:O:493:ARG:HA	1.84	0.42
1:A:353:VAL:O	1:A:354:GLN:HB2	2.19	0.42
1:B:571:THR:N	1:B:572:PRO:CD	2.83	0.42
1:C:149:ARG:HG2	1:C:149:ARG:NH1	2.34	0.42
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.01	0.42
1:D:573:LYS:HB3	1:D:573:LYS:HE3	1.89	0.42
2:M:138:ASP:N	2:M:139:PRO:CD	2.83	0.42
2:M:702:GLU:H	2:M:702:GLU:HG3	1.30	0.42
2:N:583:CYS:CB	2:N:586:THR:HG22	2.50	0.42
2:P:315:LYS:HE3	10:P:1084:HOH:O	2.19	0.42
1:B:149:ARG:HD2	10:B:1427:HOH:O	2.19	0.42
1:B:298:MET:HE1	1:B:402:ARG:CG	2.50	0.42
1:C:213:SER:HB3	1:D:209:HIS:CD2	2.55	0.42
1:C:577[A]:VAL:HG21	1:C:645:ILE:CG2	2.41	0.42
2:M:339:TYR:HB2	2:M:432:LYS:HA	2.02	0.42
2:M:568:ASN:ND2	2:M:581:GLN:HE21	2.14	0.42
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.55	0.42
2:N:377:PRO:HG2	2:N:380:SER:HB3	2.00	0.42
2:O:345:ASN:OD1	2:O:345:ASN:C	2.61	0.42
2:O:631:LEU:O	2:O:635:ILE:HG23	2.19	0.42
2:P:117[B]:ARG:NH1	10:P:1004:HOH:O	2.44	0.42
2:P:431:SER:O	2:P:435:VAL:HG23	2.19	0.42
2:P:604:ILE:HD12	2:P:610:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:HIS:CE1	1:C:416:ARG:CB	3.00	0.42
1:C:482:LEU:HD22	1:C:482:LEU:HA	1.81	0.42
1:D:12:ARG:HB3	1:D:13:PRO:HD2	2.02	0.42
2:M:7:ILE:CD1	2:M:245:ARG:HD2	2.43	0.42
2:M:587:LEU:HD23	2:M:588:MET:HE1	2.01	0.42
2:N:71:GLU:HG2	2:N:82:ILE:HD11	2.02	0.42
2:N:361:ILE:HD13	2:N:391:TYR:HB3	2.01	0.42
2:N:374:ASP:O	2:N:375:GLN:HG3	2.20	0.42
2:N:468:PHE:HB2	2:N:474:VAL:CG2	2.50	0.42
2:N:674:LEU:HD22	2:N:678:LEU:HG	2.01	0.42
1:B:78:ILE:HD11	1:B:97:ILE:HD12	2.01	0.42
1:B:218:GLN:HE22	1:B:233:SER:CB	2.32	0.42
1:C:274:ASP:HB3	1:C:308:LYS:HD3	2.02	0.42
1:D:271:LEU:HD21	1:D:331:VAL:HG11	2.02	0.42
1:D:626:ASP:HB3	2:P:212:PHE:CG	2.55	0.42
2:O:298:TYR:HA	2:O:301:ILE:HG13	2.01	0.42
2:O:581:GLN:O	2:O:590:ASN:HB3	2.20	0.42
2:O:627:THR:O	2:O:628:PHE:C	2.63	0.42
2:P:542:ILE:HG13	2:P:543:ASN:N	2.35	0.42
2:P:579:LEU:HD23	2:P:579:LEU:HA	1.90	0.42
2:P:728:ILE:HG23	2:P:728:ILE:O	2.20	0.42
2:M:333:ILE:HD12	2:M:418:TRP:CB	2.50	0.41
2:M:424:ASN:H	2:M:424:ASN:ND2	2.14	0.41
2:O:488:ARG:O	2:O:490:ASP:N	2.52	0.41
2:O:584:LEU:O	2:O:585:TYR:CD2	2.72	0.41
2:P:17:GLU:HA	2:P:18:PRO:HD3	1.93	0.41
2:P:422:GLN:HG2	2:P:423:ARG:HG3	2.02	0.41
2:P:594:SER:HB3	2:P:598:PHE:HD2	1.85	0.41
2:P:601:ILE:HG21	2:P:631:LEU:HG	2.01	0.41
1:C:414:SER:C	1:C:416:ARG:N	2.75	0.41
1:D:33:VAL:HG13	1:D:339:LEU:CD1	2.49	0.41
1:D:510:LEU:H	1:D:510:LEU:CD1	2.31	0.41
2:M:419:HIS:ND1	2:M:419:HIS:C	2.78	0.41
2:N:146:ILE:HD11	3:N:900:SF4:S1	2.60	0.41
2:N:459:ILE:HD12	2:N:542:ILE:HG13	2.02	0.41
2:O:363:ASP:HB2	2:O:462:ARG:HG2	2.03	0.41
2:O:422:GLN:N	2:O:422:GLN:CD	2.78	0.41
2:O:422:GLN:O	2:O:423:ARG:C	2.62	0.41
2:O:474:VAL:CG1	2:O:475:LYS:N	2.83	0.41
2:P:500:VAL:O	2:P:553:LYS:NZ	2.47	0.41
2:P:541:GLU:H	2:P:541:GLU:HG2	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:OG1	1:A:201:HIS:HD2	2.03	0.41
1:A:217:ASN:O	1:A:223:MET:HG3	2.21	0.41
1:C:221:MET:SD	1:C:221:MET:C	3.03	0.41
1:D:615:LEU:H	5:D:863:GOL:H12	1.84	0.41
2:M:277:ILE:HG23	2:M:295:VAL:HG23	2.02	0.41
2:O:167:LYS:HG2	10:O:997:HOH:O	2.20	0.41
2:O:315:LYS:HB2	2:O:316:ILE:H	1.50	0.41
2:O:430:VAL:CG1	2:O:431:SER:H	2.32	0.41
2:O:552:PRO:O	2:O:554:GLU:N	2.49	0.41
2:O:671:PRO:HA	2:O:702:GLU:OE1	2.20	0.41
2:P:392:GLY:HA3	2:P:459:ILE:O	2.20	0.41
2:P:505:SER:CB	2:P:570:TYR:HE2	2.31	0.41
2:P:704:ILE:HG22	2:P:711:ILE:HG22	2.02	0.41
1:B:186:LEU:CD2	1:B:205:PRO:HD2	2.50	0.41
1:D:69:ARG:HD3	1:D:75:PRO:HG3	2.02	0.41
2:M:21:LEU:HB2	2:M:286:LYS:HA	2.03	0.41
2:N:16:LYS:HZ3	2:N:16:LYS:HB3	1.85	0.41
2:N:156:GLU:HG3	2:N:182:MET:HB3	2.02	0.41
2:N:696:ILE:HA	2:N:699:ILE:HD12	2.02	0.41
2:O:95:ASN:HD21	2:O:98:ASN:H	1.67	0.41
2:O:249:ARG:HA	2:O:309:ARG:NH2	2.36	0.41
2:O:388:VAL:HG22	2:O:465:VAL:HG13	2.01	0.41
2:O:427:TRP:CE2	2:O:429:ARG:NH2	2.88	0.41
2:O:527:LEU:HD22	2:O:594:SER:HA	2.00	0.41
2:P:221:TYR:O	2:P:222:ALA:C	2.61	0.41
1:C:577[A]:VAL:HG12	1:C:601:PRO:HG2	2.01	0.41
1:D:510:LEU:O	1:D:543:PRO:HD2	2.21	0.41
2:O:348:PRO:CG	2:O:475:LYS:HE3	2.46	0.41
2:O:728:ILE:O	2:O:729:MET:O	2.38	0.41
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.87	0.41
1:C:61:ILE:HG22	1:C:67:CYS:HB2	2.02	0.41
1:C:169:LYS:O	1:C:172:GLU:HB2	2.21	0.41
1:D:51:ARG:O	1:D:52:PHE:C	2.62	0.41
2:O:343:GLY:C	2:O:349:ALA:HB2	2.44	0.41
2:O:360:GLU:O	2:O:361:ILE:CG2	2.68	0.41
2:O:396:GLN:CD	2:O:399:PHE:CD1	2.99	0.41
2:O:712:LEU:O	2:O:715:LEU:N	2.54	0.41
2:P:478:MET:O	2:P:482:ARG:HB2	2.20	0.41
1:A:284:ASN:HD22	1:A:284:ASN:C	2.29	0.41
1:B:368:HIS:NE2	1:B:416:ARG:CD	2.84	0.41
1:B:398:LYS:O	1:B:402:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:ILE:HG23	1:C:597:SER:OG	2.21	0.41
2:N:350:PHE:HA	2:N:423:ARG:O	2.20	0.41
2:O:243:TYR:CD1	2:O:243:TYR:C	2.98	0.41
2:O:482:ARG:O	2:O:485:TYR:HB3	2.20	0.41
2:P:254:TYR:O	2:P:278:THR:HA	2.21	0.41
2:P:581:GLN:O	2:P:590:ASN:HB3	2.20	0.41
1:B:467:ILE:O	1:B:497:ALA:HA	2.20	0.41
1:C:507:LYS:HB2	1:C:507:LYS:HE3	1.87	0.41
1:D:186:LEU:HD22	1:D:205:PRO:HD2	2.03	0.41
2:M:315:LYS:O	2:M:316:ILE:O	2.38	0.41
2:M:683:VAL:HG13	2:M:693:GLU:HA	2.03	0.41
2:O:343:GLY:C	2:O:347:THR:O	2.64	0.41
2:O:482:ARG:O	2:O:485:TYR:CB	2.69	0.41
1:D:149[B]:ARG:HD2	1:D:188:THR:O	2.20	0.41
2:M:169:LEU:HD13	2:M:193:LEU:HD21	2.03	0.41
2:O:344:GLY:N	2:O:426:ASN:O	2.54	0.41
2:O:488:ARG:NH1	2:O:488:ARG:CG	2.83	0.41
2:O:489:ASP:OD1	2:O:489:ASP:C	2.63	0.41
2:O:604:ILE:CD1	2:O:606:PRO:HD3	2.30	0.41
2:O:661:ASP:O	2:O:666:ARG:NE	2.32	0.41
2:P:656:LYS:HA	2:P:656:LYS:HD3	1.81	0.41
1:A:78:ILE:HD11	1:A:97:ILE:HD12	2.03	0.41
1:A:587:LYS:H	1:B:220:HIS:HE1	1.68	0.41
1:B:601:PRO:HB3	1:B:631:TYR:CZ	2.56	0.41
1:C:313:VAL:HG12	1:C:329:PRO:HG2	2.02	0.41
2:O:187:ASP:HA	2:O:211:ASN:HD22	1.85	0.41
2:O:726:ASP:HB2	2:O:727:PRO:HD2	2.03	0.41
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.85	0.41
1:A:279:VAL:HG22	1:A:313:VAL:CG2	2.51	0.40
1:A:469:GLY:C	4:A:800:XCC:S1	3.04	0.40
1:C:112:ALA:HA	1:D:217:ASN:ND2	2.33	0.40
1:C:197:LYS:HE2	1:C:197:LYS:HB2	1.88	0.40
1:D:220:HIS:CD2	1:D:221:MET:O	2.72	0.40
5:D:863:GOL:C2	2:P:27:HIS:CE1	3.00	0.40
2:M:711:ILE:O	2:M:715:LEU:HG	2.20	0.40
2:N:651:TYR:HA	10:N:876:HOH:O	2.21	0.40
2:O:61:TYR:CD1	2:O:66:ARG:HD2	2.55	0.40
2:O:182:MET:HG3	2:O:205:ILE:HG22	2.01	0.40
2:O:281:PRO:HG3	2:O:296:GLU:OE2	2.21	0.40
2:O:351:GLU:CG	2:O:423:ARG:N	2.65	0.40
2:O:430:VAL:HG12	2:O:434:ALA:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:21:LEU:HB2	2:P:286:LYS:HA	2.01	0.40
2:P:494:GLY:N	10:P:1094:HOH:O	2.34	0.40
1:A:77:ARG:HB3	10:A:1466:HOH:O	2.22	0.40
1:A:235:ILE:HG23	1:A:597:SER:OG	2.21	0.40
2:O:351:GLU:O	2:O:352:LEU:CB	2.65	0.40
2:O:366:ILE:H	2:O:366:ILE:HG13	1.74	0.40
2:O:424:ASN:ND2	2:O:485:TYR:HE1	2.16	0.40
2:P:341:GLU:OE1	2:P:427:TRP:NE1	2.53	0.40
1:B:652:ARG:O	1:B:656:LEU:HB2	2.22	0.40
1:D:170:ALA:O	1:D:173:ASP:HB2	2.21	0.40
1:D:201:HIS:HE1	1:D:627:VAL:HG13	1.86	0.40
1:D:320:ASN:O	1:D:321:GLU:C	2.63	0.40
2:M:199:LYS:HE2	2:M:415:GLU:OE2	2.22	0.40
2:M:563:ILE:HD11	2:M:583:CYS:SG	2.61	0.40
2:O:111:GLU:HA	2:O:216:VAL:HG11	2.03	0.40
2:P:287:GLN:HE22	2:P:289:PRO:HG3	1.87	0.40
2:P:427:TRP:C	2:P:428:LEU:HD12	2.46	0.40
1:B:662:VAL:HG21	2:N:194:LEU:HD13	2.03	0.40
1:C:174:PHE:CE2	1:C:208:ILE:HD12	2.56	0.40
1:D:116:HIS:CD2	1:D:116:HIS:C	3.00	0.40
1:D:200:THR:OG1	1:D:201:HIS:HD2	2.05	0.40
2:M:349:ALA:CB	2:M:426:ASN:HD21	2.35	0.40
2:N:604:ILE:HG13	2:N:643:GLY:O	2.21	0.40
2:O:484:LYS:HD3	2:O:484:LYS:HA	1.59	0.40
1:A:20:MET:HG3	10:A:883:HOH:O	2.21	0.40
1:A:440:LEU:HB3	1:A:448:PRO:O	2.21	0.40
1:C:384:TYR:HE2	2:P:88:ALA:HB2	1.86	0.40
2:M:349:ALA:HB3	2:M:426:ASN:HD21	1.86	0.40
2:O:720:HIS:O	2:O:723:LEU:N	2.54	0.40
2:P:351:GLU:CD	2:P:426:ASN:HD21	2.30	0.40
2:P:442:LYS:HE2	2:P:442:LYS:HB2	1.66	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	678/674 (101%)	652 (96%)	24 (4%)	2 (0%)	36	34
1	B	676/674 (100%)	652 (96%)	23 (3%)	1 (0%)	48	50
1	C	673/674 (100%)	648 (96%)	24 (4%)	1 (0%)	48	50
1	D	675/674 (100%)	640 (95%)	30 (4%)	5 (1%)	18	13
2	M	731/729 (100%)	687 (94%)	36 (5%)	8 (1%)	11	7
2	N	732/729 (100%)	689 (94%)	34 (5%)	9 (1%)	10	5
2	O	727/729 (100%)	641 (88%)	60 (8%)	26 (4%)	2	0
2	P	727/729 (100%)	679 (93%)	41 (6%)	7 (1%)	12	8
All	All	5619/5612 (100%)	5288 (94%)	272 (5%)	59 (1%)	11	7

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ASN
1	D	267	ASN
2	M	316	ILE
2	M	693	GLU
2	O	315	LYS
2	O	316	ILE
2	O	317	LYS
2	O	361	ILE
2	O	397	ALA
2	O	482	ARG
2	O	485	TYR
2	O	486	LYS
2	O	492	MET
2	O	728	ILE
2	P	316	ILE
2	P	360	GLU
1	A	267	ASN
2	M	187	ASP
2	M	315	LYS
2	N	187	ASP
2	N	449	VAL
2	N	693	GLU
2	O	187	ASP
2	O	335	LYS

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Mol	Chain	Res	Type
2	O	470	ASP
2	O	555	GLY
2	P	458	ALA
2	P	679	HIS
1	C	267	ASN
2	M	596	GLY
2	M	658	ILE
2	O	436	ALA
2	O	489	ASP
2	O	650	THR
2	O	679	HIS
2	P	187	ASP
2	N	426	ASN
2	O	399	PHE
2	P	228	MET
2	P	596	GLY
1	A	354	GLN
1	D	552	ASP
2	N	290	ASP
2	O	459	ILE
2	O	727	PRO
1	D	354	GLN
1	D	416	ARG
1	D	492	ASN
2	M	478	MET
2	M	719	GLY
2	N	596	GLY
2	O	484	LYS
2	N	316	ILE
2	O	382	LEU
2	O	460	VAL
2	N	402	VAL
2	O	392	GLY
2	O	658	ILE
2	N	658	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	548/543 (101%)	525 (96%)	23 (4%)	26	25
1	B	547/543 (101%)	524 (96%)	23 (4%)	26	25
1	C	542/543 (100%)	519 (96%)	23 (4%)	26	25
1	D	544/543 (100%)	520 (96%)	24 (4%)	25	23
2	M	615/611 (101%)	566 (92%)	49 (8%)	11	7
2	N	615/611 (101%)	571 (93%)	44 (7%)	13	8
2	O	611/611 (100%)	510 (84%)	101 (16%)	2	1
2	P	611/611 (100%)	547 (90%)	64 (10%)	6	3
All	All	4633/4616 (100%)	4282 (92%)	351 (8%)	12	8

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	140	GLU
1	A	153	GLU
1	A	159	VAL
1	A	206	PHE
1	A	284	ASN
1	A	298	MET
1	A	303	LYS
1	A	318	THR
1	A	415	ASN
1	A	418	VAL
1	A	426	ARG
1	A	427	VAL
1	A	438	LYS
1	A	466	LEU
1	A	482	LEU
1	A	518	THR
1	A	538	GLU
1	A	647	ASP
1	A	656	LEU
1	A	664	GLU
1	A	665[A]	ARG
1	A	665[B]	ARG
1	B	66	ILE
1	B	77	ARG

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Mol	Chain	Res	Type
1	B	120	ILE
1	B	148[A]	ARG
1	B	148[B]	ARG
1	B	153	GLU
1	B	159	VAL
1	B	206	PHE
1	B	308	LYS
1	B	318	THR
1	B	389	GLN
1	B	395	GLU
1	B	411	ARG
1	B	413	GLU
1	B	447	ASN
1	B	466	LEU
1	B	467	ILE
1	B	482	LEU
1	B	518	THR
1	B	537	ILE
1	B	600	VAL
1	B	647	ASP
1	B	656	LEU
1	C	23	LYS
1	C	27	ARG
1	C	81	THR
1	C	82	ASP
1	C	153	GLU
1	C	159	VAL
1	C	206	PHE
1	C	318	THR
1	C	323	LEU
1	C	359	SER
1	C	390	THR
1	C	395	GLU
1	C	418	VAL
1	C	466	LEU
1	C	467	ILE
1	C	482	LEU
1	C	539	ILE
1	C	600	VAL
1	C	639	GLN
1	C	647	ASP
1	C	656	LEU

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Mol	Chain	Res	Type
1	C	664	GLU
1	C	669	LYS
1	D	45	VAL
1	D	66	ILE
1	D	153	GLU
1	D	159	VAL
1	D	190	ILE
1	D	196	GLU
1	D	199	ARG
1	D	206	PHE
1	D	284	ASN
1	D	291	ILE
1	D	293	GLN
1	D	298	MET
1	D	299	GLU
1	D	331	VAL
1	D	413	GLU
1	D	423	ILE
1	D	427	VAL
1	D	466	LEU
1	D	467	ILE
1	D	470	CYS
1	D	594	TRP
1	D	600	VAL
1	D	656	LEU
1	D	664	GLU
2	M	6[A]	LYS
2	M	6[B]	LYS
2	M	14	GLU
2	M	66	ARG
2	M	125	GLU
2	M	169	LEU
2	M	198	VAL
2	M	199	LYS
2	M	214	GLN
2	M	215	ILE
2	M	245	ARG
2	M	249	ARG
2	M	262	LYS
2	M	314	THR
2	M	315	LYS
2	M	316	ILE

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Mol	Chain	Res	Type
2	M	317	LYS
2	M	318	LEU
2	M	332	SER
2	M	335	LYS
2	M	342	MET
2	M	354	ARG
2	M	373	ILE
2	M	376	ILE
2	M	380	SER
2	M	409	ASP
2	M	422	GLN
2	M	424	ASN
2	M	426	ASN
2	M	448	LEU
2	M	469	THR
2	M	475	LYS
2	M	486	LYS
2	M	539	SER
2	M	565	LYS
2	M	571	LEU
2	M	604	ILE
2	M	607	GLU
2	M	654	SER
2	M	672	LYS
2	M	674	LEU
2	M	681[A]	GLU
2	M	681[B]	GLU
2	M	684	ARG
2	M	694	ASP
2	M	702	GLU
2	M	704	ILE
2	M	724	THR
2	M	726	ASP
2	N	6	LYS
2	N	66	ARG
2	N	124	ASP
2	N	125	GLU
2	N	146	ILE
2	N	152	THR
2	N	174[A]	LYS
2	N	174[B]	LYS
2	N	198	VAL

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Mol	Chain	Res	Type
2	N	205	ILE
2	N	245	ARG
2	N	249	ARG
2	N	312	LYS
2	N	313	LEU
2	N	315	LYS
2	N	316	ILE
2	N	331	GLU
2	N	335	LYS
2	N	338	MET
2	N	354	ARG
2	N	358	GLU
2	N	373	ILE
2	N	386	ILE
2	N	388	VAL
2	N	405	ARG
2	N	424	ASN
2	N	425	ILE
2	N	440	ARG
2	N	448	LEU
2	N	471	GLU
2	N	492	MET
2	N	495	LEU
2	N	560	ILE
2	N	571	LEU
2	N	604	ILE
2	N	606	PRO
2	N	631	LEU
2	N	635	ILE
2	N	640	GLN
2	N	674	LEU
2	N	681	GLU
2	N	686	SER
2	N	693	GLU
2	N	702	GLU
2	O	6	LYS
2	O	17	GLU
2	O	39	LEU
2	O	64	VAL
2	O	66	ARG
2	O	71	GLU
2	O	95	ASN

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Mol	Chain	Res	Type
2	O	125	GLU
2	O	127	LEU
2	O	149	VAL
2	O	152	THR
2	O	166	SER
2	O	169	LEU
2	O	174	LYS
2	O	185	ILE
2	O	198	VAL
2	O	205	ILE
2	O	214	GLN
2	O	216	VAL
2	O	233	THR
2	O	238	GLU
2	O	245	ARG
2	O	246	ARG
2	O	313	LEU
2	O	314	THR
2	O	315	LYS
2	O	316	ILE
2	O	317	LYS
2	O	318	LEU
2	O	322	ILE
2	O	333	ILE
2	O	335	LYS
2	O	339	TYR
2	O	342	MET
2	O	350	PHE
2	O	351	GLU
2	O	352	LEU
2	O	366	ILE
2	O	367	GLU
2	O	368	VAL
2	O	376	ILE
2	O	391	TYR
2	O	395	MET
2	O	404	GLU
2	O	407	ILE
2	O	411	ILE
2	O	426	ASN
2	O	427	TRP
2	O	428	LEU

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Mol	Chain	Res	Type
2	O	429	ARG
2	O	432	LYS
2	O	448	LEU
2	O	449	VAL
2	O	453	LYS
2	O	454	GLU
2	O	459	ILE
2	O	463	VAL
2	O	467	ILE
2	O	478	MET
2	O	480	VAL
2	O	482	ARG
2	O	484	LYS
2	O	487	GLU
2	O	488	ARG
2	O	491	ARG
2	O	492	MET
2	O	493	ARG
2	O	495	LEU
2	O	497	ASP
2	O	499	THR
2	O	500	VAL
2	O	502	THR
2	O	511	SER
2	O	524	ARG
2	O	541	GLU
2	O	542	ILE
2	O	556	GLU
2	O	567	VAL
2	O	573	THR
2	O	575	SER
2	O	579	LEU
2	O	580	GLU
2	O	592	MET
2	O	608	CYS
2	O	612	MET
2	O	621	MET
2	O	631	LEU
2	O	641	THR
2	O	647	ILE
2	O	659	SER
2	O	672	LYS

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Mol	Chain	Res	Type
2	O	683	VAL
2	O	686	SER
2	O	687	VAL
2	O	691	LEU
2	O	693	GLU
2	O	696	ILE
2	O	697	ASP
2	O	708	VAL
2	O	723	LEU
2	O	729	MET
2	P	39	LEU
2	P	64	VAL
2	P	66	ARG
2	P	120	LYS
2	P	124	ASP
2	P	125	GLU
2	P	152	THR
2	P	166	SER
2	P	174	LYS
2	P	175	GLU
2	P	198	VAL
2	P	199	LYS
2	P	205	ILE
2	P	238	GLU
2	P	245	ARG
2	P	284	GLU
2	P	300	LYS
2	P	301	ILE
2	P	312	LYS
2	P	317	LYS
2	P	331	GLU
2	P	332	SER
2	P	335	LYS
2	P	341	GLU
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	351	GLU
2	P	354	ARG
2	P	362	THR
2	P	369	ILE
2	P	373	ILE

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Mol	Chain	Res	Type
2	P	394	LYS
2	P	398	ASP
2	P	403	LEU
2	P	404	GLU
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	442	LYS
2	P	448	LEU
2	P	462	ARG
2	P	467	ILE
2	P	469	THR
2	P	480	VAL
2	P	482	ARG
2	P	483	GLU
2	P	486	LYS
2	P	500	VAL
2	P	502	THR
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	549	GLN
2	P	553	LYS
2	P	557	ILE
2	P	581	GLN
2	P	605	LEU
2	P	631	LEU
2	P	674	LEU
2	P	686	SER
2	P	717	GLU
2	P	726	ASP
2	P	729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	164	GLN
1	A	201	HIS
1	A	209	HIS
1	A	217	ASN
1	A	218	GLN

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Mol	Chain	Res	Type
1	A	220	HIS
1	A	284	ASN
1	A	471	ASN
1	A	477	GLN
1	A	479	ASN
1	A	503	GLN
1	A	515	ASN
1	B	9	HIS
1	B	122	HIS
1	B	201	HIS
1	B	209	HIS
1	B	217	ASN
1	B	218	GLN
1	B	220	HIS
1	B	260	GLN
1	B	275	GLN
1	B	293	GLN
1	B	454	GLN
1	B	477	GLN
1	B	565	ASN
1	B	672	GLN
1	C	9	HIS
1	C	201	HIS
1	C	209	HIS
1	C	217	ASN
1	C	218	GLN
1	C	220	HIS
1	C	275	GLN
1	C	368	HIS
1	C	454	GLN
1	C	477	GLN
1	C	503	GLN
1	C	515	ASN
1	C	622	GLN
1	C	639	GLN
1	C	672	GLN
1	D	201	HIS
1	D	209	HIS
1	D	217	ASN
1	D	218	GLN
1	D	220	HIS
1	D	284	ASN

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Mol	Chain	Res	Type
1	D	293	GLN
1	D	477	GLN
1	D	622	GLN
1	D	639	GLN
2	M	211	ASN
2	M	287	GLN
2	M	375	GLN
2	M	408	HIS
2	M	424	ASN
2	M	426	ASN
2	M	544	HIS
2	M	581	GLN
2	M	590	ASN
2	N	211	ASN
2	N	345	ASN
2	N	396	GLN
2	N	408	HIS
2	N	424	ASN
2	N	510	GLN
2	N	581	GLN
2	N	590	ASN
2	N	640	GLN
2	O	27	HIS
2	O	95	ASN
2	O	211	ASN
2	O	244	GLN
2	O	419	HIS
2	O	515	ASN
2	O	516	HIS
2	O	568	ASN
2	O	576	ASN
2	O	590	ASN
2	O	618	HIS
2	O	640	GLN
2	P	27	HIS
2	P	211	ASN
2	P	287	GLN
2	P	396	GLN
2	P	408	HIS
2	P	422	GLN
2	P	424	ASN
2	P	426	ASN

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Mol	Chain	Res	Type
2	P	443	ASN
2	P	516	HIS
2	P	549	GLN
2	P	578	ASN
2	P	581	GLN
2	P	590	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 12 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	A	750	1	0,12,12	-	-	-		
3	SF4	O	900	2	0,12,12	-	-	-		
4	XCC	B	800	10,1	0,12,12	-	-	-		
3	SF4	D	750	1	0,12,12	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
3	SF4	N	900	2	0,12,12	-	-	-		
5	GOL	C	863	-	5,5,5	0.31	0	5,5,5	0.65	0
8	ACT	P	953	-	1,2,3	1.54	0	0,1,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	863	-	5,5,5	1.10	1 (20%)	5,5,5	1.85	1 (20%)
4	XCC	D	800	10,1	0,12,12	-	-	-	-	-
8	ACT	O	953	-	1,2,3	1.23	0	0,1,3	-	-
3	SF4	A	700	1	0,12,12	-	-	-	-	-
3	SF4	C	700	1	0,12,12	-	-	-	-	-
5	GOL	A	863	-	5,5,5	0.45	0	5,5,5	1.82	2 (40%)
5	GOL	D	863	-	5,5,5	0.54	0	5,5,5	1.72	2 (40%)
4	XCC	A	800	10,1	0,12,12	-	-	-	-	-
8	ACT	N	953	-	1,2,3	1.45	0	0,1,3	-	-
8	ACT	M	953	-	1,2,3	1.35	0	0,1,3	-	-
4	XCC	C	800	10,1	0,12,12	-	-	-	-	-
3	SF4	C	750	1	0,12,12	-	-	-	-	-
3	SF4	M	900	2	0,12,12	-	-	-	-	-
3	SF4	P	900	2	0,12,12	-	-	-	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	C	750	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
3	SF4	M	900	2	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
4	XCC	A	800	10,1	-	-	0/4/4/4
4	XCC	C	800	10,1	-	-	0/4/4/4
4	XCC	D	800	10,1	-	-	0/4/4/4
4	XCC	B	800	10,1	-	-	0/4/4/4
3	SF4	D	750	1	-	-	0/6/5/5
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	N	900	2	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
5	GOL	C	863	-	-	2/4/4/4	-
3	SF4	C	700	1	-	-	0/6/5/5
5	GOL	A	863	-	-	2/4/4/4	-
5	GOL	B	863	-	-	0/4/4/4	-
5	GOL	D	863	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	863	GOL	O2-C2	-2.41	1.36	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	863	GOL	O2-C2-C3	-3.29	95.57	109.18
5	D	863	GOL	O1-C1-C2	-2.87	97.45	110.38
5	A	863	GOL	O1-C1-C2	-2.49	99.16	110.38
5	A	863	GOL	O3-C3-C2	-2.06	101.10	110.38
5	D	863	GOL	O2-C2-C1	-2.01	100.86	109.18

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

10 monomers are involved in 21 short contacts:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	673/674 (99%)	-0.26	2 (0%)	90 91	14, 25, 43, 60	7 (1%)
1	B	673/674 (99%)	-0.39	8 (1%)	76 79	11, 22, 39, 68	5 (0%)
1	C	673/674 (99%)	-0.17	1 (0%)	92 93	15, 28, 42, 58	2 (0%)
1	D	673/674 (99%)	-0.01	3 (0%)	88 90	13, 31, 45, 59	4 (0%)
2	M	728/729 (99%)	0.18	23 (3%)	50 54	12, 33, 62, 74	5 (0%)
2	N	728/729 (99%)	0.22	57 (7%)	19 21	10, 32, 66, 76	6 (0%)
2	O	728/729 (99%)	1.61	261 (35%)	1 1	26, 64, 92, 126	1 (0%)
2	P	728/729 (99%)	0.66	84 (11%)	9 10	15, 45, 76, 92	1 (0%)
All	All	5604/5612 (99%)	0.25	439 (7%)	19 21	10, 31, 74, 126	31 (0%)

All (439) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	312[A]	LYS	6.6
2	O	728	ILE	6.4
2	O	458	ALA	5.9
2	O	428	LEU	5.9
2	O	495	LEU	5.8
2	O	683	VAL	5.5
2	O	397	ALA	5.5
2	O	480	VAL	5.3
2	O	691	LEU	5.3
2	O	457	PRO	5.2
2	O	647	ILE	5.2
2	O	366	ILE	5.2
2	O	481	ALA	5.0
1	B	539	ILE	5.0
2	O	574	ALA	5.0
2	O	353	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	O	567	VAL	5.0
2	O	449	VAL	4.8
2	O	474	VAL	4.8
2	O	316	ILE	4.8
2	O	339	TYR	4.7
2	N	480	VAL	4.7
2	O	344	GLY	4.7
2	N	486[A]	LYS	4.6
2	O	425	ILE	4.6
2	O	472	ALA	4.5
2	O	369	ILE	4.5
2	O	724	THR	4.5
2	O	463	VAL	4.5
2	O	450	ALA	4.5
2	O	368	VAL	4.4
2	O	488	ARG	4.4
2	O	542	ILE	4.4
2	O	361	ILE	4.3
2	O	340	VAL	4.2
2	O	348	PRO	4.2
2	O	477	TYR	4.2
2	O	570	TYR	4.2
2	N	468	PHE	4.2
2	O	399	PHE	4.2
2	O	467	ILE	4.2
2	O	356	VAL	4.2
2	O	460	VAL	4.2
2	O	525	VAL	4.2
2	O	427	TRP	4.2
2	O	485	TYR	4.1
2	O	465	VAL	4.1
2	O	579	LEU	4.1
2	O	552	PRO	4.1
2	O	355	THR	4.1
2	O	377	PRO	4.0
2	O	382	LEU	4.0
1	B	416	ARG	4.0
2	O	350	PHE	4.0
2	O	708	VAL	4.0
2	O	352	LEU	3.9
2	O	534	LEU	3.9
2	O	687	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
2	N	348	PRO	3.9
2	O	468	PHE	3.9
1	A	415	ASN	3.9
2	P	356	VAL	3.8
2	O	722	ALA	3.8
2	O	402	VAL	3.8
2	O	484	LYS	3.8
2	O	545	ALA	3.8
2	P	495	LEU	3.8
2	O	494	GLY	3.8
2	O	469	THR	3.7
2	O	380	SER	3.7
2	O	723	LEU	3.7
2	N	481	ALA	3.7
2	O	700	ALA	3.7
2	O	383	PRO	3.7
2	N	729	MET	3.7
2	O	459	ILE	3.7
2	O	595	CYS	3.6
2	O	388	VAL	3.6
2	O	390	ILE	3.6
2	O	560	ILE	3.6
2	O	593	THR	3.6
2	N	474	VAL	3.6
2	O	531	VAL	3.6
2	P	474	VAL	3.6
2	O	557	ILE	3.6
2	O	486	LYS	3.6
2	M	316	ILE	3.6
2	O	587	LEU	3.6
2	O	482	ARG	3.6
2	O	526	GLY	3.6
2	O	322	ILE	3.5
2	O	386	ILE	3.5
2	O	551	ILE	3.5
2	P	728	ILE	3.5
2	N	387	LEU	3.5
2	O	417	LEU	3.5
2	O	471	GLU	3.5
2	P	425	ILE	3.5
2	O	364	GLY	3.5
2	M	314	THR	3.5

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Mol	Chain	Res	Type	RSRZ
2	M	640[A]	GLN	3.5
2	O	373	ILE	3.5
2	O	519	ILE	3.5
2	O	665	ALA	3.5
2	O	540	TYR	3.5
2	O	473	LYS	3.5
2	P	353	VAL	3.5
2	O	314	THR	3.5
2	P	316	ILE	3.4
2	O	407	ILE	3.4
2	O	362	THR	3.4
2	N	316	ILE	3.4
2	O	639	THR	3.3
2	P	496	THR	3.3
2	O	572	TYR	3.3
2	O	559	PRO	3.3
2	O	696	ILE	3.3
2	P	350	PHE	3.3
2	O	563	ILE	3.3
2	O	667	ILE	3.3
2	M	318	LEU	3.3
2	N	318	LEU	3.3
2	O	387	LEU	3.3
2	O	470	ASP	3.3
2	O	496	THR	3.3
2	O	544	HIS	3.3
2	O	376	ILE	3.3
2	P	428	LEU	3.3
2	O	645	MET	3.3
2	P	729	MET	3.3
2	O	389	ASP	3.3
2	O	547	PRO	3.2
2	M	458	ALA	3.2
2	N	361	ILE	3.2
2	O	699	ILE	3.2
2	O	384	LEU	3.2
2	N	650	THR	3.2
2	O	686	SER	3.2
2	O	478	MET	3.2
2	O	492	MET	3.2
2	O	394	LYS	3.2
2	O	504	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	P	639	THR	3.2
2	N	315	LYS	3.2
2	O	442	LYS	3.2
2	O	655	LYS	3.2
2	O	729	MET	3.2
2	O	714	TYR	3.2
2	O	711	ILE	3.1
2	O	664	ILE	3.1
2	O	347	THR	3.1
2	O	420	THR	3.1
2	O	456	PHE	3.1
2	O	682	PHE	3.1
2	O	430	VAL	3.1
1	B	537	ILE	3.1
2	P	336	GLY	3.1
2	O	713	PRO	3.1
2	P	486	LYS	3.1
2	O	678	LEU	3.1
2	O	564	TRP	3.0
2	O	444	TYR	3.0
2	O	491	ARG	3.0
2	P	481	ALA	3.0
2	O	447	ILE	3.0
2	P	333	ILE	3.0
2	O	346	ARG	3.0
2	O	663	GLY	3.0
2	M	729	MET	3.0
2	O	395	MET	3.0
2	O	333	ILE	3.0
2	O	707	THR	3.0
1	D	417	PRO	3.0
2	O	371	PRO	3.0
2	P	559	PRO	3.0
2	O	451	LYS	3.0
2	O	421	GLY	3.0
2	P	339	TYR	3.0
2	O	594	SER	2.9
2	O	345	ASN	2.9
2	P	579	LEU	2.9
2	N	638	GLY	2.9
2	O	553	LYS	2.9
2	N	362	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	O	670	MET	2.9
2	O	436	ALA	2.9
2	O	583	CYS	2.9
2	O	650	THR	2.9
2	N	383	PRO	2.9
2	O	317	LYS	2.9
2	N	472	ALA	2.9
2	O	712	LEU	2.9
2	O	601	ILE	2.9
2	O	613	ILE	2.9
2	O	391	TYR	2.9
2	P	683	VAL	2.8
2	P	355	THR	2.8
2	N	390	ILE	2.8
2	O	475	LYS	2.8
2	O	503	PHE	2.8
2	P	418	TRP	2.8
2	O	641	THR	2.8
2	N	376	ILE	2.8
2	N	360	GLU	2.8
2	N	434	ALA	2.8
2	M	382	LEU	2.8
2	O	466	THR	2.8
2	O	573	THR	2.8
2	O	653	VAL	2.8
2	O	721	PRO	2.8
2	P	427	TRP	2.8
2	P	623	PRO	2.8
2	O	431	SER	2.8
2	N	466	THR	2.8
2	O	586	THR	2.8
2	M	728	ILE	2.8
2	N	366	ILE	2.8
2	O	354	ARG	2.7
2	O	441	PHE	2.7
2	P	477	TYR	2.7
2	P	584	LEU	2.7
2	O	500	VAL	2.7
2	O	418	TRP	2.7
2	O	497	ASP	2.7
2	O	637	GLY	2.7
2	O	365	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	660	ALA	2.7
2	O	403	LEU	2.7
1	B	443	GLN	2.7
2	N	369	ILE	2.7
2	O	715	LEU	2.7
2	P	320	LEU	2.7
2	P	715	LEU	2.7
2	O	623	PRO	2.7
2	O	652	ILE	2.7
2	P	369	ILE	2.7
2	N	545	ALA	2.6
2	O	499	THR	2.6
2	O	657	PHE	2.6
2	M	345	ASN	2.6
2	N	384	LEU	2.6
2	P	552	PRO	2.6
2	N	300[A]	LYS	2.6
2	N	368	VAL	2.6
2	O	435	VAL	2.6
2	O	507	VAL	2.6
2	P	583	CYS	2.6
2	M	481	ALA	2.6
2	N	458	ALA	2.6
2	P	700	ALA	2.6
2	M	313	LEU	2.6
2	O	401	GLY	2.6
2	O	662	GLY	2.6
2	P	492	MET	2.6
2	O	426	ASN	2.6
2	O	632	ALA	2.6
2	N	495	LEU	2.6
2	O	396	GLN	2.6
2	P	407	ILE	2.6
2	O	336	GLY	2.6
2	P	478	MET	2.6
2	O	381	LYS	2.6
2	P	475	LYS	2.6
2	P	484	LYS	2.6
2	O	434	ALA	2.6
2	O	359	SER	2.6
2	O	571	LEU	2.6
2	P	712	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	M	376	ILE	2.5
2	N	728	ILE	2.5
2	O	611	ILE	2.5
2	O	668	VAL	2.5
2	N	370	GLY	2.5
2	O	648	GLY	2.5
2	O	530	ALA	2.5
2	O	606	PRO	2.5
2	N	350	PHE	2.5
2	O	695	PHE	2.5
2	N	373	ILE	2.5
2	N	388	VAL	2.5
2	O	627	THR	2.5
2	O	619	ALA	2.5
2	O	674	LEU	2.5
2	P	387	LEU	2.5
2	O	533	TRP	2.5
2	N	317	LYS	2.5
2	N	463	VAL	2.5
2	M	124	ASP	2.5
2	M	693	GLU	2.5
2	N	367	GLU	2.5
2	O	566	SER	2.5
2	M	371	PRO	2.5
2	O	612	MET	2.5
1	D	368	HIS	2.5
2	O	335	LYS	2.5
2	P	335	LYS	2.5
2	M	467	ILE	2.5
2	N	467	ILE	2.5
2	P	359	SER	2.4
2	P	362	THR	2.4
2	O	318	LEU	2.4
2	O	605	LEU	2.4
2	M	343	GLY	2.4
2	O	385	GLY	2.4
2	O	638	GLY	2.4
2	O	520	VAL	2.4
2	O	704	ILE	2.4
2	O	669	TRP	2.4
2	N	377	PRO	2.4
2	O	602	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	488	ARG	2.4
2	P	491	ARG	2.4
1	B	536	ASN	2.4
2	O	582	VAL	2.4
2	P	460	VAL	2.4
2	O	634	MET	2.4
1	D	669[A]	LYS	2.4
2	O	502	THR	2.4
2	P	482	ARG	2.4
2	P	713	PRO	2.4
2	P	727	PRO	2.4
1	B	538	GLU	2.4
2	O	476	GLU	2.4
2	O	562	GLY	2.4
2	O	719	GLY	2.4
2	P	555	GLY	2.4
2	O	229	PHE	2.4
2	O	635	ILE	2.4
2	P	340	VAL	2.4
2	P	480	VAL	2.4
2	P	493	ARG	2.4
1	A	368	HIS	2.4
2	N	639	THR	2.4
2	P	485	TYR	2.3
2	M	472	ALA	2.3
2	O	689	GLU	2.3
2	N	313	LEU	2.3
2	O	448	LEU	2.3
2	O	392	GLY	2.3
2	P	373	ILE	2.3
2	P	402	VAL	2.3
2	N	485	TYR	2.3
2	N	382	LEU	2.3
2	O	313	LEU	2.3
2	P	313	LEU	2.3
2	P	723	LEU	2.3
2	N	124	ASP	2.3
2	O	124	ASP	2.3
2	N	492	MET	2.3
2	O	342	MET	2.3
2	P	361	ILE	2.3
2	N	371	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	424	ASN	2.3
2	M	637	GLY	2.3
2	N	392	GLY	2.3
2	N	477	TYR	2.3
2	O	585	TYR	2.3
2	N	425	ILE	2.3
2	P	376	ILE	2.3
2	O	522	PRO	2.3
2	O	727	PRO	2.3
2	M	315	LYS	2.3
2	O	432	LYS	2.3
2	P	562	GLY	2.3
2	P	638	GLY	2.3
2	P	342	MET	2.3
2	O	151	TRP	2.3
2	O	679	HIS	2.2
2	O	410	PHE	2.2
2	P	459	ILE	2.2
2	P	377	PRO	2.2
2	O	538	ALA	2.2
2	P	397	ALA	2.2
2	N	391	TYR	2.2
2	O	13	PRO	2.2
2	O	604	ILE	2.2
2	O	642	PRO	2.2
2	P	420	THR	2.2
2	P	557	ILE	2.2
2	O	584	LEU	2.2
2	O	631	LEU	2.2
2	P	572	TYR	2.2
2	O	698	LYS	2.2
2	P	371	PRO	2.2
2	O	343	GLY	2.2
2	O	516	HIS	2.2
2	O	518	CYS	2.2
2	P	571	LEU	2.2
2	P	570	TYR	2.2
2	O	615	THR	2.2
2	O	716	GLU	2.1
2	P	483	GLU	2.1
2	O	517	VAL	2.1
2	O	506	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	505	SER	2.1
2	M	477	TYR	2.1
2	O	558	ASP	2.1
2	O	614	THR	2.1
2	P	457	PRO	2.1
2	P	560	ILE	2.1
2	P	664	ILE	2.1
2	O	600	ALA	2.1
2	O	357	SER	2.1
2	N	469	THR	2.1
2	O	423	ARG	2.1
2	O	546	GLY	2.1
2	O	658	ILE	2.1
2	N	465	VAL	2.1
2	O	338	MET	2.1
2	O	725	MET	2.1
2	N	314	THR	2.1
2	P	385	GLY	2.1
1	C	539	ILE	2.1
2	M	390	ILE	2.1
2	O	146	ILE	2.1
2	O	512	PHE	2.1
2	P	533	TRP	2.1
1	B	155	GLU	2.0
2	O	532	SER	2.1
2	O	659	SER	2.1
2	O	452	MET	2.0
2	O	588	MET	2.0
2	P	403	LEU	2.0
2	O	576	ASN	2.0
2	N	389	ASP	2.0
2	P	501	ASP	2.0
2	O	493	ARG	2.0
2	M	724	THR	2.0
2	N	473	LYS	2.0
2	O	561	LYS	2.0
2	P	394	LYS	2.0
2	P	432	LYS	2.0
1	B	540	GLY	2.0
2	P	682	PHE	2.0
2	O	654	SER	2.0
2	P	357	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	490	ASP	2.0
2	O	694	ASP	2.0
2	O	651	TYR	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
5	GOL	C	863	6/6	0.77	0.17	47,56,56,58	0
9	NA	O	730	1/1	0.86	0.10	70,70,70,70	0
5	GOL	D	863	6/6	0.87	0.13	43,46,48,48	0
9	NA	P	730	1/1	0.87	0.08	35,35,35,35	0
8	ACT	N	953	3/4	0.89	0.21	59,59,59,59	0
8	ACT	P	953	3/4	0.90	0.21	53,53,54,54	0
8	ACT	M	953	3/4	0.93	0.15	44,44,44,45	0
5	GOL	A	863	6/6	0.93	0.10	26,30,33,37	0
8	ACT	O	953	3/4	0.93	0.23	100,100,100,100	0
3	SF4	O	900	8/8	0.94	0.07	61,63,67,67	0
5	GOL	B	863	6/6	0.96	0.08	26,30,34,37	0
6	CU1	P	950	1/1	0.96	0.05	55,55,55,55	0
9	NA	M	730	1/1	0.97	0.05	29,29,29,29	0
9	NA	N	730	1/1	0.97	0.03	28,28,28,28	0
6	CU1	O	950	1/1	0.97	0.04	82,82,82,82	0
7	NI	O	951	1/1	0.97	0.06	76,76,76,76	0
3	SF4	C	700	8/8	0.98	0.04	28,32,35,35	0
3	SF4	P	900	8/8	0.98	0.04	40,40,41,46	0
4	XCC	C	800	9/9	0.98	0.04	25,27,34,35	0
6	CU1	N	950	1/1	0.99	0.04	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SF4	A	750	8/8	0.99	0.03	14,17,17,18	0
3	SF4	B	750	8/8	0.99	0.03	17,18,18,19	0
7	NI	M	951	1/1	0.99	0.02	28,28,28,28	0
4	XCC	A	800	9/9	0.99	0.03	20,24,29,30	0
7	NI	P	951	1/1	0.99	0.04	39,39,39,39	0
4	XCC	B	800	9/9	0.99	0.03	16,20,25,27	0
3	SF4	A	700	8/8	0.99	0.03	17,19,20,22	0
4	XCC	D	800	9/9	0.99	0.03	33,35,41,45	0
3	SF4	C	750	8/8	0.99	0.03	28,30,31,32	0
3	SF4	D	750	8/8	0.99	0.05	26,28,29,29	0
3	SF4	M	900	8/8	0.99	0.03	22,25,26,28	0
3	SF4	N	900	8/8	0.99	0.03	25,26,27,28	0
6	CU1	M	950	1/1	0.99	0.03	43,43,43,43	0
7	NI	N	951	1/1	1.00	0.01	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.