



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 02:46 PM EDT

PDB ID : 3I04 / pdb_00003i04
Title : Cyanide-bound structure of bifunctional carbon monoxide dehydrogenase/acetate-CoA synthase from Moorella thermoacetica, cyanide-bound C-cluster
Authors : Kung, Y.; Doukov, T.I.; Drennan, C.L.
Deposited on : 2009-06-24
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

<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

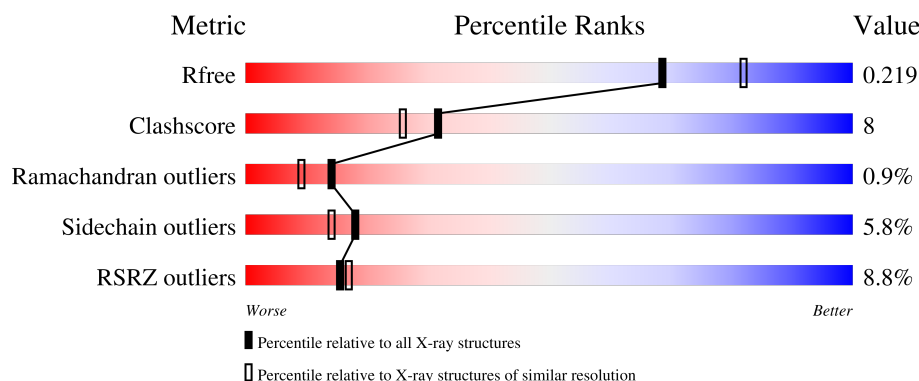
1 Overall quality at a glance

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	673	88% 11% .
1	B	673	87% 12% .
1	C	673	89% 10%
1	D	673	87% 12% .
2	M	728	85% 12% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CYN	A	900	-	-	X	-
5	CYN	C	900	-	-	X	-
6	GOL	C	963	-	-	X	-
6	GOL	D	963	-	-	X	-
9	ACT	N	953	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 45801 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

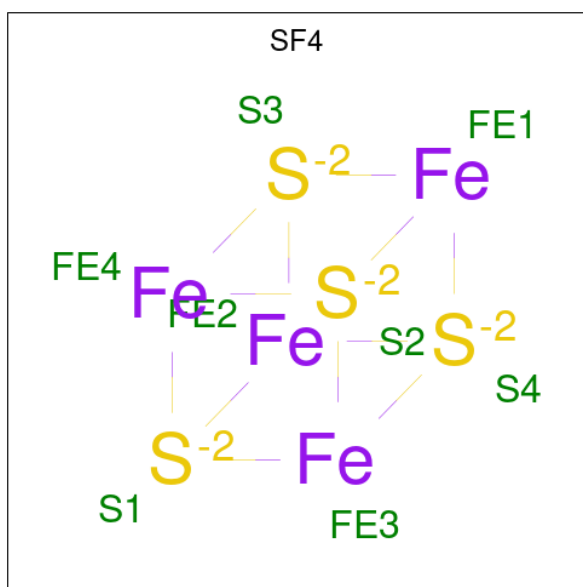
- Molecule 1 is a protein called Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta.

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

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

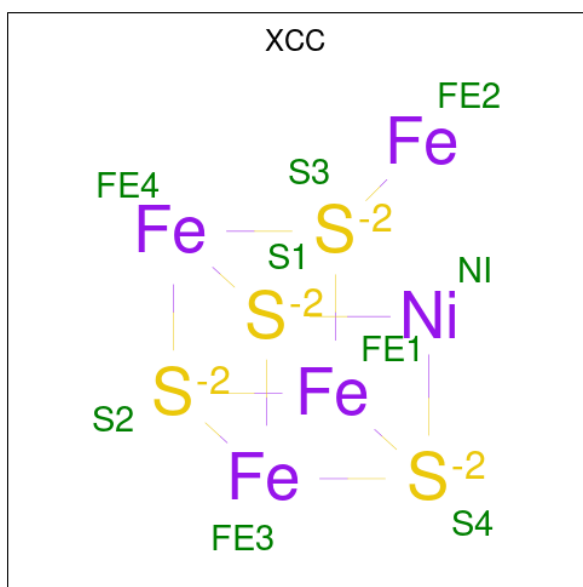
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	728	Total	C	N	O	S	0	4	0
			5766	3695	962	1074	35			
2	N	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	O	728	Total	C	N	O	S	0	1	0
			5746	3684	959	1068	35			
2	P	728	Total	C	N	O	S	0	2	0
			5757	3690	963	1069	35			

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



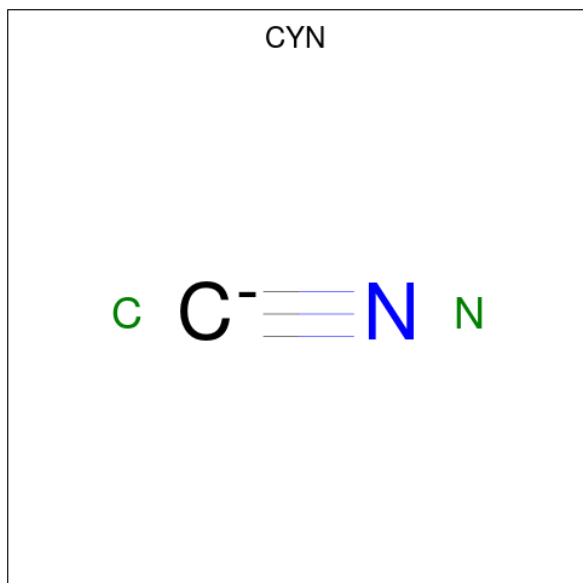
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	D	1	Total	Fe	S	0	0
			8	4	4		
3	M	1	Total	Fe	S	0	0
			8	4	4		
3	N	1	Total	Fe	S	0	0
			8	4	4		
3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



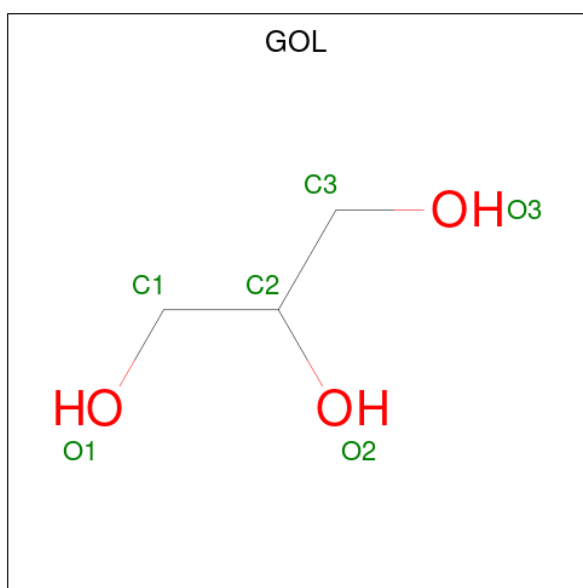
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
4	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

- Molecule 5 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

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

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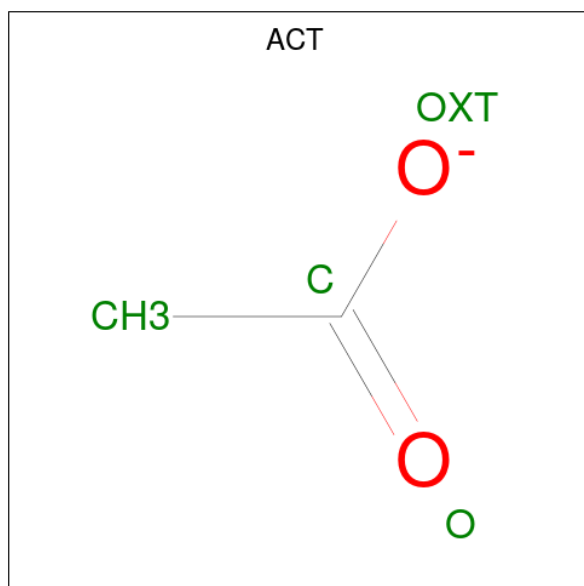
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	1	Total	Cu	0	0
			1	1		
7	P	1	Total	Cu	0	0
			1	1		

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

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

- Molecule 10 is SODIUM ION (CCD ID: NA) (formula: Na).

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

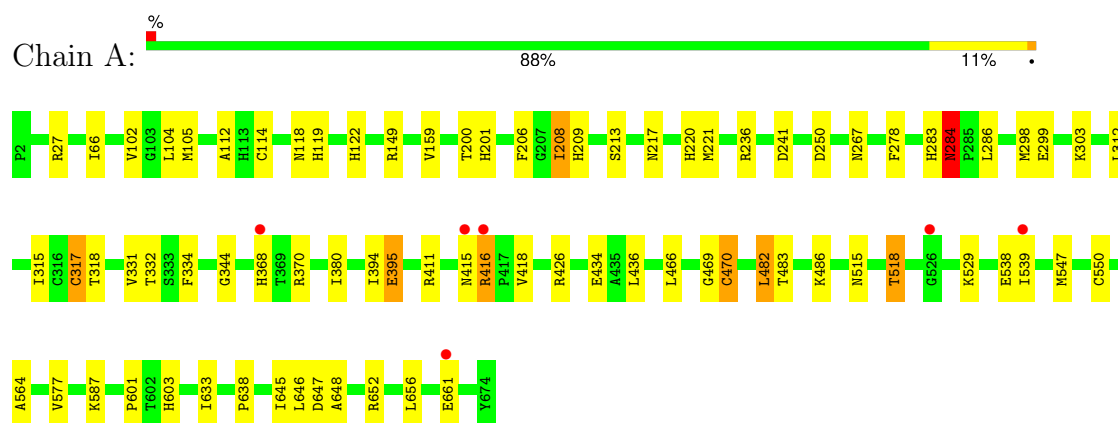
- Molecule 11 is water.

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

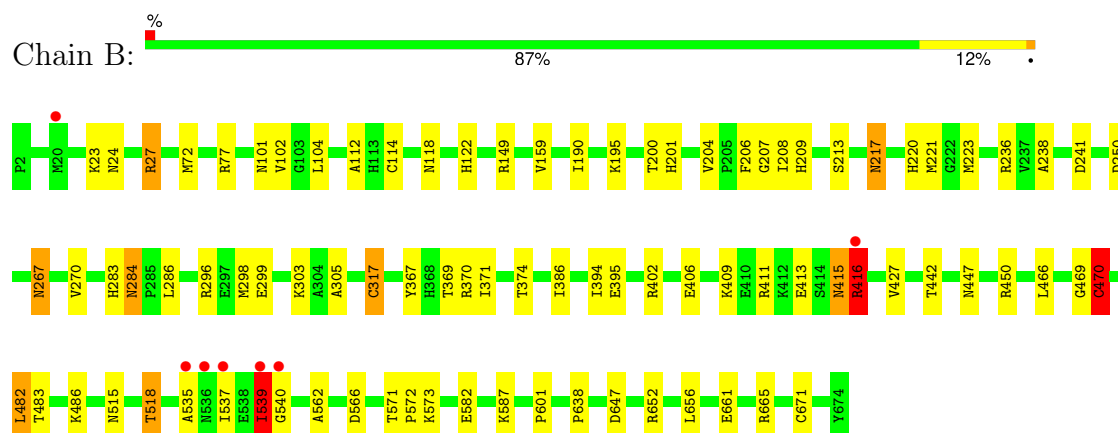
3 Residue-property plots

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.

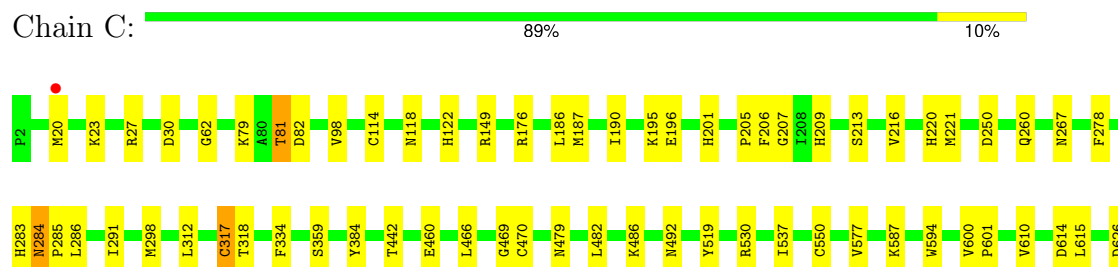
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta



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

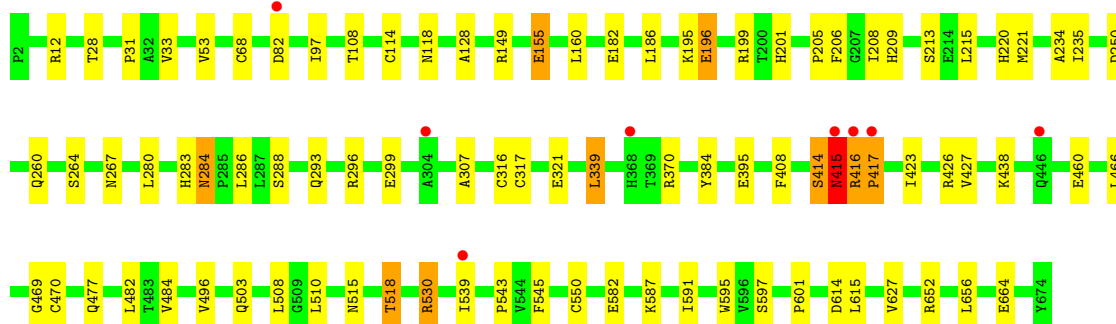
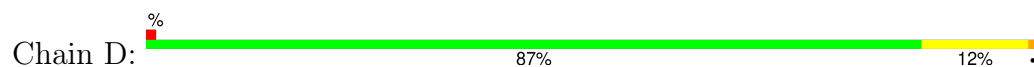


- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

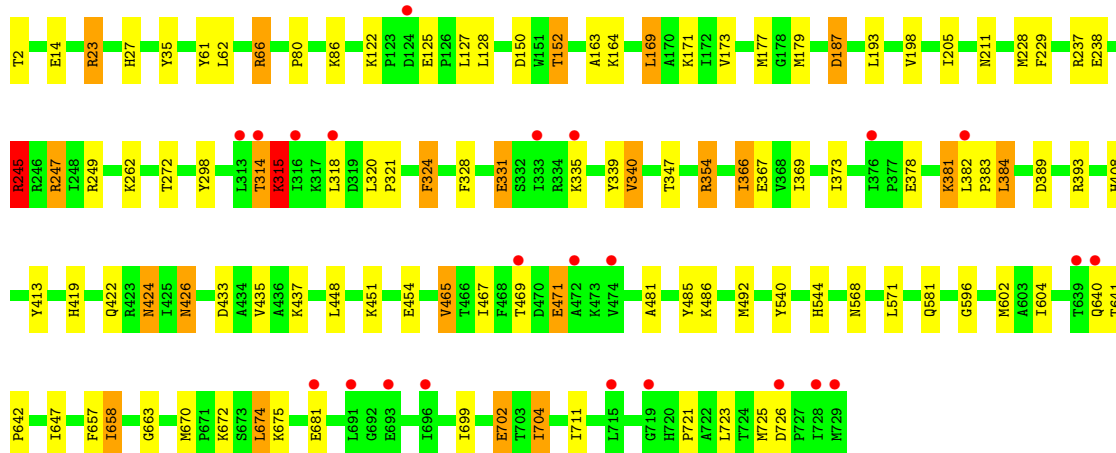
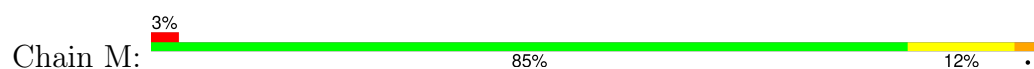




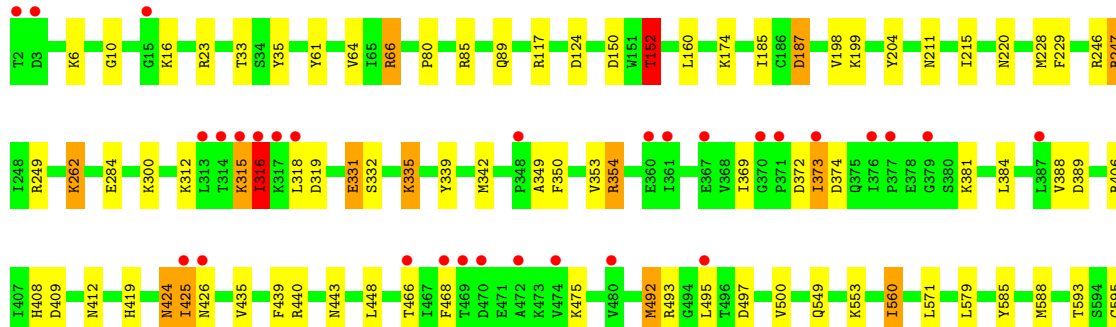
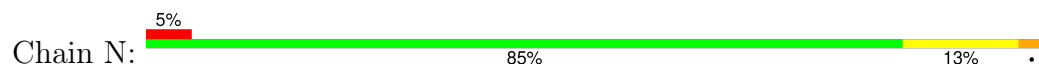
- Molecule 1: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit beta

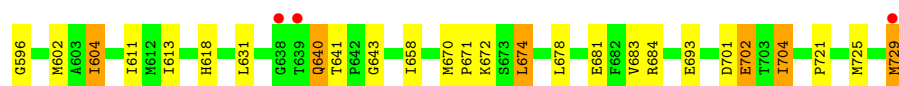


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

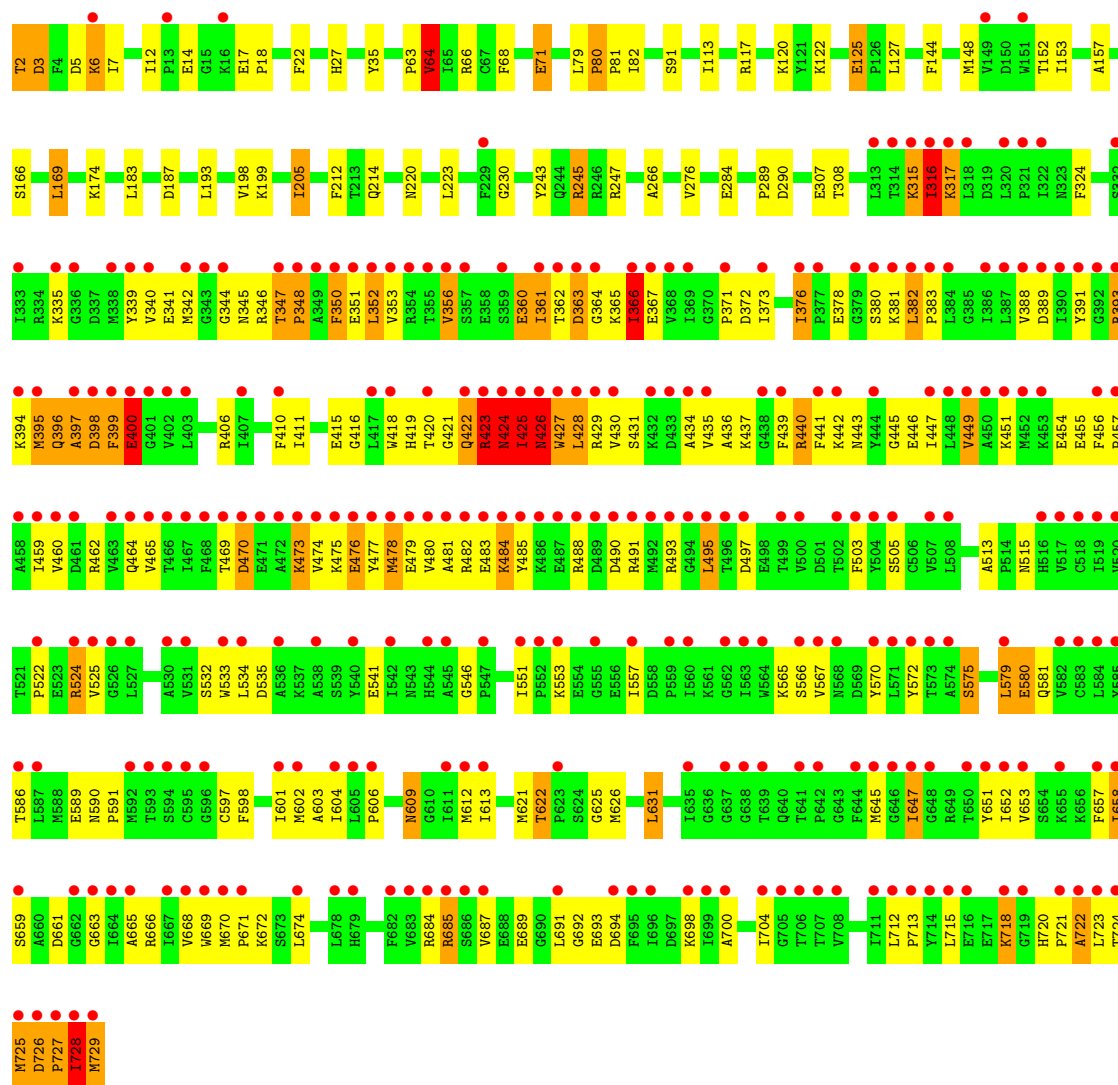
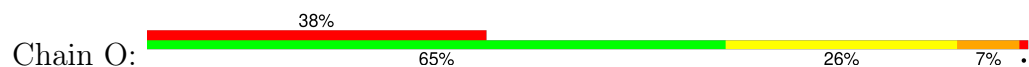


- Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha

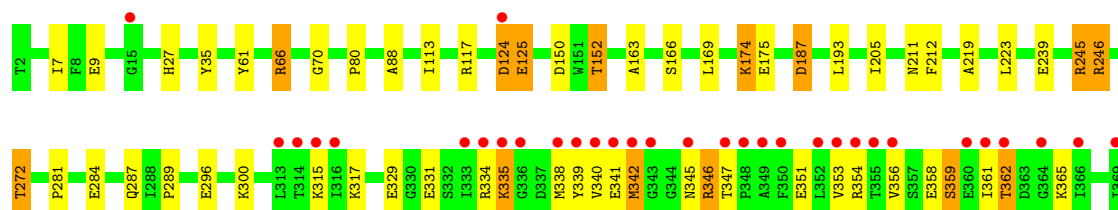
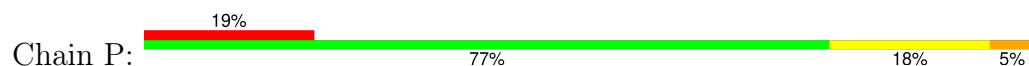


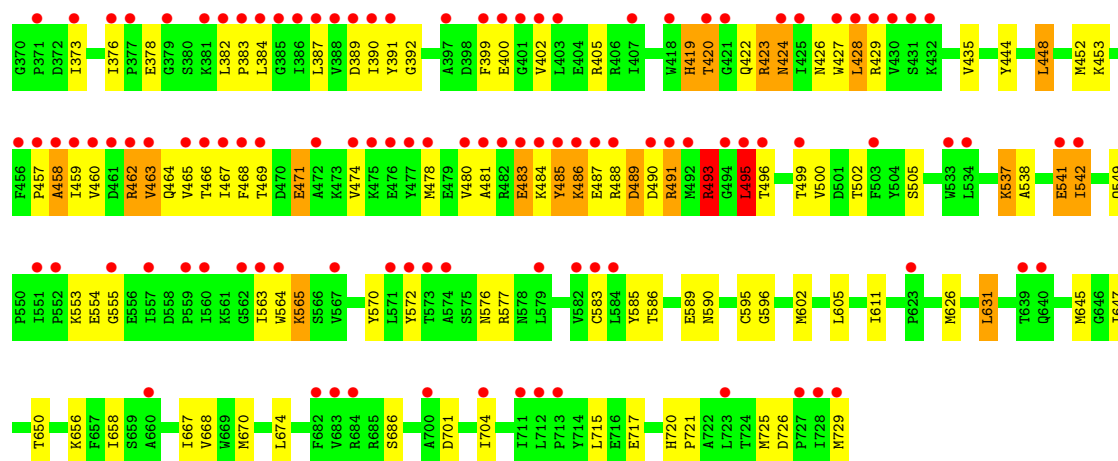


● Molecule 2: Carbon monoxide dehydrogenase/acetyl-CoA synthase subunit alpha



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





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.83Å 136.77Å 141.61Å 101.23° 109.18° 103.87°	Depositor
Resolution (Å)	48.39 – 2.15 48.39 – 2.15	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.39-2.15) 96.5 (48.39-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.31 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.221 0.172 , 0.219	Depositor DCC
R_{free} test set	17112 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45801	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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: SF4, NI, ACT, GOL, XCC, CYN, CU1, NA

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	1.23	5/5230 (0.1%)	1.10	15/7086 (0.2%)
1	B	1.24	11/5244 (0.2%)	1.08	9/7105 (0.1%)
1	C	1.15	1/5200 (0.0%)	1.08	10/7048 (0.1%)
1	D	1.12	7/5181 (0.1%)	1.09	4/7021 (0.1%)
2	M	1.10	8/5909 (0.1%)	1.06	7/8000 (0.1%)
2	N	1.09	4/5885 (0.1%)	1.05	6/7968 (0.1%)
2	O	0.98	11/5885 (0.2%)	1.09	20/7968 (0.3%)
2	P	0.95	3/5896 (0.1%)	1.03	14/7982 (0.2%)
All	All	1.11	50/44430 (0.1%)	1.07	85/60178 (0.1%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	425	ILE	CA-CB	-9.76	1.45	1.55
2	O	400	GLU	CA-C	-8.92	1.40	1.52
1	D	414	SER	CA-C	-8.74	1.41	1.52
1	D	414	SER	C-O	-8.12	1.12	1.24
2	O	425	ILE	CG1-CD1	-7.75	1.21	1.51
1	D	155	GLU	CA-C	-7.73	1.42	1.52
2	O	425	ILE	CA-C	-7.71	1.43	1.52
2	M	198	VAL	C-O	-7.63	1.14	1.24
2	N	85	ARG	C-O	7.36	1.32	1.24
2	P	420	THR	C-O	-7.30	1.14	1.23
1	A	469	GLY	CA-C	-6.93	1.42	1.51
1	D	264	SER	C-O	-6.86	1.19	1.24
1	B	647	ASP	C-O	-6.66	1.16	1.24
1	B	236	ARG	CA-C	6.58	1.61	1.52
1	A	564	ALA	CA-CB	6.46	1.63	1.53
2	M	324	PHE	C-O	-6.42	1.16	1.23
2	M	198	VAL	N-CA	-6.21	1.38	1.46
2	N	641	THR	CA-CB	6.20	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	155	GLU	C-N	-6.15	1.25	1.33
1	B	539	ILE	CA-CB	6.12	1.61	1.54
1	A	236	ARG	CA-C	6.04	1.60	1.52
2	M	23	ARG	C-O	-6.00	1.17	1.24
1	A	102	VAL	CA-CB	5.98	1.62	1.54
2	M	465	VAL	CA-CB	5.95	1.62	1.54
1	A	648	ALA	CA-CB	5.89	1.62	1.53
2	O	423	ARG	N-CA	-5.74	1.38	1.46
1	B	369	THR	C-O	-5.73	1.17	1.23
1	B	406	GLU	C-O	-5.73	1.17	1.24
1	D	196	GLU	C-O	-5.62	1.17	1.24
1	B	562	ALA	CA-CB	5.57	1.61	1.53
1	C	469	GLY	CA-C	-5.51	1.45	1.52
2	M	62	LEU	N-CA	5.50	1.52	1.46
2	O	64	VAL	CA-CB	5.47	1.62	1.54
2	P	212	PHE	C-O	-5.42	1.19	1.24
2	O	428	LEU	C-O	5.42	1.30	1.23
2	O	424	ASN	N-CA	-5.40	1.39	1.46
2	O	382	LEU	CA-C	5.38	1.59	1.52
1	B	102	VAL	CA-CB	5.34	1.61	1.54
1	B	371	ILE	CA-CB	5.33	1.60	1.54
2	O	476	GLU	C-O	5.27	1.30	1.24
2	P	80	PRO	CA-C	5.25	1.57	1.52
2	M	245	ARG	CA-C	5.21	1.59	1.52
1	B	207	GLY	CA-C	5.19	1.56	1.52
2	N	33	THR	CA-CB	5.17	1.61	1.53
1	B	469	GLY	C-O	-5.15	1.16	1.23
2	M	366	ILE	CA-CB	5.14	1.61	1.54
2	N	152	THR	C-O	-5.11	1.17	1.24
1	B	159	VAL	C-O	-5.09	1.18	1.24
2	O	153	ILE	N-CA	5.08	1.50	1.46
1	D	484	VAL	CA-CB	5.07	1.60	1.54

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	398	ASP	CA-C-N	-9.29	110.77	122.84
2	O	398	ASP	C-N-CA	-9.29	110.77	122.84
1	B	470	CYS	N-CA-C	8.90	121.22	110.19
2	O	477	TYR	N-CA-C	-8.69	102.69	113.20
1	A	470	CYS	N-CA-C	8.63	122.26	110.35
2	P	493	ARG	N-CA-C	-8.46	102.06	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	476	GLU	CA-C-O	8.40	129.63	119.97
1	B	317	CYS	N-CA-C	7.48	119.52	111.36
2	P	485	TYR	N-CA-C	7.44	119.03	111.07
2	O	400	GLU	N-CA-C	-6.95	95.99	110.80
1	A	344	GLY	N-CA-C	-6.87	106.22	115.36
1	D	469	GLY	N-CA-C	6.79	124.38	112.83
2	P	420	THR	N-CA-C	-6.78	97.20	108.32
2	M	314	THR	N-CA-C	-6.70	103.77	112.68
1	C	334	PHE	N-CA-C	6.67	119.16	111.02
2	O	428	LEU	N-CA-C	-6.47	100.39	110.17
2	O	425	ILE	O-C-N	-6.46	117.35	122.97
2	O	80	PRO	N-CA-C	6.31	118.40	110.70
2	O	580	GLU	N-CA-C	6.25	123.05	112.99
2	M	80	PRO	N-CA-C	6.23	118.30	110.70
2	O	91	SER	CA-C-N	6.22	126.33	119.87
2	O	91	SER	C-N-CA	6.22	126.33	119.87
2	P	670	MET	CA-C-N	-6.19	113.60	119.85
2	P	670	MET	C-N-CA	-6.19	113.60	119.85
2	O	513	ALA	CA-C-N	6.15	127.53	119.84
2	O	513	ALA	C-N-CA	6.15	127.53	119.84
1	C	284	ASN	CB-CA-C	6.08	116.19	110.17
2	P	428	LEU	N-CA-C	6.00	118.41	108.99
2	P	485	TYR	CB-CA-C	-5.93	101.57	110.88
1	C	469	GLY	N-CA-C	5.90	123.23	112.37
1	B	204	VAL	CA-C-N	-5.86	113.90	119.76
1	B	204	VAL	C-N-CA	-5.86	113.90	119.76
1	A	434	GLU	N-CA-C	-5.84	104.92	111.28
1	B	101	ASN	N-CA-C	5.82	117.42	111.14
1	C	317	CYS	N-CA-C	5.80	117.69	111.36
2	M	237	ARG	N-CA-C	5.79	117.26	111.07
2	N	80	PRO	N-CA-C	5.78	117.75	110.70
1	A	208	ILE	N-CA-C	5.71	115.78	110.42
1	A	380	ILE	CA-C-N	-5.64	113.97	119.78
1	A	380	ILE	C-N-CA	-5.64	113.97	119.78
2	P	246	ARG	N-CA-C	5.63	117.10	111.07
2	O	546	GLY	CA-C-N	5.60	125.70	119.87
2	O	546	GLY	C-N-CA	5.60	125.70	119.87
2	M	128	LEU	CA-C-N	-5.58	114.63	120.38
2	M	128	LEU	C-N-CA	-5.58	114.63	120.38
1	A	284	ASN	CA-C-N	-5.57	114.08	119.87
1	A	284	ASN	C-N-CA	-5.57	114.08	119.87
1	B	469	GLY	N-CA-C	5.56	122.59	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	412	ASN	N-CA-C	5.49	117.98	111.33
2	N	670	MET	CA-C-N	-5.47	114.32	119.85
2	N	670	MET	C-N-CA	-5.47	114.32	119.85
1	C	470	CYS	N-CA-C	5.47	118.33	109.79
1	D	12	ARG	CA-C-N	-5.47	114.96	120.21
1	D	12	ARG	C-N-CA	-5.47	114.96	120.21
1	C	594	TRP	N-CA-C	5.42	118.11	111.82
1	A	469	GLY	CA-C-N	5.42	132.06	121.66
1	A	469	GLY	C-N-CA	5.42	132.06	121.66
2	N	425	ILE	CA-C-N	5.39	128.89	120.75
2	N	425	ILE	C-N-CA	5.39	128.89	120.75
2	P	491	ARG	CA-C-O	-5.36	114.04	120.10
1	C	30	ASP	CA-C-N	-5.34	114.16	119.56
1	C	30	ASP	C-N-CA	-5.34	114.16	119.56
1	D	591	ILE	N-CA-C	5.34	115.97	110.36
1	C	318	THR	N-CA-C	-5.34	105.62	111.82
2	O	68	PHE	N-CA-C	5.33	119.50	112.89
2	P	80	PRO	N-CA-C	5.32	117.19	110.70
2	M	384	LEU	N-CA-C	5.32	117.84	108.75
2	O	426	ASN	CA-C-N	-5.32	111.39	121.54
2	O	426	ASN	C-N-CA	-5.32	111.39	121.54
2	P	495	LEU	N-CA-C	5.28	116.93	107.80
2	O	424	ASN	N-CA-C	-5.27	103.76	111.30
1	B	217	ASN	N-CA-C	5.25	116.69	111.07
2	P	166	SER	N-CA-C	5.25	116.68	111.07
1	A	334	PHE	N-CA-C	5.24	119.96	111.37
2	M	331	GLU	N-CA-C	5.19	116.99	110.24
1	A	66	ILE	N-CA-C	5.17	117.09	112.17
1	A	317	CYS	N-CA-C	5.16	116.98	111.36
2	O	475	LYS	O-C-N	-5.16	115.09	122.41
2	P	423	ARG	CB-CA-C	-5.15	110.62	116.54
1	A	646	LEU	CA-C-N	5.15	127.43	120.38
1	A	646	LEU	C-N-CA	5.15	127.43	120.38
1	C	492	ASN	N-CA-C	5.11	118.79	112.24
1	B	416	ARG	CA-C-N	-5.07	115.01	120.03
1	B	416	ARG	C-N-CA	-5.07	115.01	120.03
2	P	392	GLY	N-CA-C	-5.02	102.22	110.80

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	5134	0	5139	60	0
1	B	5134	0	5133	66	0
1	C	5103	0	5090	50	0
1	D	5088	0	5086	61	0
2	M	5766	0	5723	63	0
2	N	5746	0	5710	66	0
2	O	5746	0	5711	242	0
2	P	5757	0	5722	129	0
3	A	16	0	0	0	0
3	B	8	0	0	0	0
3	C	16	0	0	1	0
3	D	8	0	0	0	0
3	M	8	0	0	0	0
3	N	8	0	0	0	0
3	O	8	0	0	0	0
3	P	8	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
5	A	2	0	0	2	0
5	B	2	0	0	0	0
5	C	2	0	0	3	0
5	D	2	0	0	1	0
6	A	6	0	8	1	0
6	B	6	0	8	0	0
6	C	6	0	8	4	0
6	D	6	0	8	6	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	M	3	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	3	0	3	3	0
9	O	3	0	3	1	0
9	P	3	0	3	1	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
11	A	306	0	0	5	0
11	B	375	0	0	5	0
11	C	275	0	0	6	0
11	D	240	0	0	5	0
11	M	326	0	0	5	0
11	N	337	0	0	9	0
11	O	83	0	0	1	0
11	P	213	0	0	3	0
All	All	45801	0	43358	707	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (707) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MET:HE1	1:B:72:MET:CG	1.54	1.37
2:O:425:ILE:HD12	2:O:425:ILE:C	1.47	1.32
1:B:370:ARG:HD2	11:B:1495:HOH:O	1.33	1.28
2:O:425:ILE:HD12	2:O:426:ASN:N	1.48	1.28
2:O:395:MET:SD	2:O:399:PHE:HE2	1.57	1.27
1:A:105:MET:CE	1:B:72:MET:HG3	1.69	1.23
2:O:425:ILE:O	2:O:426:ASN:ND2	1.81	1.14
2:O:482:ARG:HD2	2:O:485:TYR:OH	1.44	1.13
2:O:478:MET:HE3	2:O:478:MET:HA	1.15	1.11
2:O:490:ASP:O	2:O:493:ARG:HG2	1.48	1.10
1:D:416:ARG:CB	1:D:417:PRO:HD2	1.81	1.08
2:O:395:MET:SD	2:O:399:PHE:CE2	2.48	1.07
2:O:482:ARG:HA	2:O:485:TYR:CE2	1.90	1.06
2:P:338:MET:CE	2:P:341:GLU:HB2	1.86	1.06
2:O:346:ARG:NH2	2:O:427:TRP:CZ2	2.23	1.06
2:O:728:ILE:HG23	2:O:728:ILE:O	1.56	1.05
2:O:424:ASN:O	2:O:425:ILE:HG22	1.57	1.04
2:O:395:MET:HA	2:O:399:PHE:CZ	1.93	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:391:TYR:HB3	2:P:462:ARG:NH1	1.74	1.03
2:O:657:PHE:CE1	2:O:658:ILE:HD12	1.95	1.02
2:O:425:ILE:C	2:O:426:ASN:ND2	2.17	1.01
2:O:426:ASN:O	2:O:427:TRP:HB2	1.19	1.01
2:O:426:ASN:O	2:O:427:TRP:CB	2.05	1.00
2:P:354:ARG:HD2	2:P:356:VAL:HG13	1.44	1.00
2:P:400:GLU:OE2	2:P:484:LYS:HE3	1.62	0.99
1:D:416:ARG:CB	1:D:417:PRO:CD	2.38	0.98
2:M:602:MET:HE2	2:M:657:PHE:HE2	1.31	0.95
1:D:114:CYS:HB2	11:D:1014:HOH:O	1.66	0.95
2:O:346:ARG:NH1	2:O:427:TRP:CZ2	2.36	0.94
2:O:622:THR:HG23	2:O:626:MET:O	1.68	0.92
2:M:602:MET:HE2	2:M:657:PHE:CE2	2.04	0.92
2:O:395:MET:HA	2:O:399:PHE:CE2	2.06	0.91
2:P:362:THR:H	2:P:464:GLN:HE21	1.18	0.91
2:M:602:MET:HE3	2:M:647:ILE:HG21	1.52	0.90
2:O:425:ILE:CD1	2:O:426:ASN:N	2.34	0.89
2:O:478:MET:HA	2:O:478:MET:CE	2.00	0.88
2:P:602:MET:HE2	2:P:647:ILE:HG21	1.56	0.88
2:P:400:GLU:OE2	2:P:484:LYS:CE	2.23	0.87
2:P:338:MET:HE2	2:P:341:GLU:HB2	1.55	0.87
1:C:114:CYS:HB2	11:C:1383:HOH:O	1.74	0.86
2:O:478:MET:HE3	2:O:478:MET:CA	2.02	0.86
2:O:316:ILE:CG2	2:O:454:GLU:HG3	2.07	0.84
2:O:346:ARG:HH22	2:O:427:TRP:HZ2	1.23	0.84
2:O:482:ARG:HD2	2:O:485:TYR:HH	1.42	0.84
2:O:482:ARG:HA	2:O:485:TYR:CZ	2.13	0.84
2:O:481:ALA:O	2:O:485:TYR:CD2	2.31	0.83
2:P:483:GLU:OE2	2:P:483:GLU:HA	1.77	0.83
2:O:346:ARG:NH2	2:O:427:TRP:CH2	2.43	0.82
1:C:122:HIS:HD2	11:C:905:HOH:O	1.60	0.82
2:P:602:MET:HE1	2:P:645:MET:HE3	1.62	0.82
1:A:105:MET:HE1	1:B:72:MET:HG3	0.82	0.81
2:P:354:ARG:HD2	2:P:356:VAL:CG1	2.11	0.81
2:P:342:MET:HG3	2:P:384:LEU:HD22	1.63	0.80
2:O:425:ILE:O	2:O:426:ASN:CB	2.24	0.80
2:O:728:ILE:O	2:O:728:ILE:CG2	2.30	0.80
2:O:346:ARG:CZ	2:O:427:TRP:CZ2	2.64	0.79
2:P:338:MET:HE3	2:P:429:ARG:HE	1.46	0.79
2:P:424:ASN:H	2:P:424:ASN:HD22	1.30	0.79
2:O:490:ASP:O	2:O:493:ARG:CG	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:229:PHE:CD1	9:N:953:ACT:H2	2.18	0.79
1:D:182:GLU:OE2	1:D:199:ARG:HD3	1.81	0.78
1:C:614:ASP:H	6:C:963:GOL:H11	1.49	0.78
1:C:550:CYS:HB3	5:C:900:CYN:N	1.99	0.78
2:O:376:ILE:HD12	2:O:382:LEU:HD21	1.63	0.77
2:O:424:ASN:O	2:O:425:ILE:CG2	2.30	0.77
1:D:466:LEU:HD22	1:D:595:TRP:CZ2	2.20	0.77
1:A:515:ASN:HD22	1:A:518:THR:HG21	1.50	0.77
2:P:338:MET:HE1	2:P:341:GLU:HB2	1.65	0.76
2:O:12:ILE:HG21	2:O:17:GLU:HG3	1.67	0.76
2:O:482:ARG:CD	2:O:485:TYR:OH	2.30	0.76
2:O:424:ASN:C	2:O:425:ILE:CG2	2.59	0.76
2:O:71:GLU:HG3	2:O:82:ILE:HD11	1.67	0.76
2:P:338:MET:HE3	2:P:429:ARG:NE	2.00	0.76
2:O:481:ALA:O	2:O:485:TYR:CE2	2.39	0.75
2:P:400:GLU:CD	2:P:484:LYS:HE3	2.12	0.75
2:O:346:ARG:NH2	2:O:427:TRP:HZ2	1.79	0.75
2:M:335:LYS:HD2	2:M:335:LYS:H	1.52	0.74
2:O:376:ILE:CD1	2:O:382:LEU:HD21	2.17	0.74
2:O:651:TYR:CD2	2:O:657:PHE:CD2	2.76	0.74
1:A:515:ASN:HD22	1:A:518:THR:CG2	2.00	0.74
2:N:354:ARG:HD2	2:N:389:ASP:OD2	1.86	0.74
2:O:726:ASP:OD2	2:O:729:MET:HB2	1.87	0.74
2:M:602:MET:HE3	2:M:647:ILE:HD13	1.69	0.74
1:C:550:CYS:CB	5:C:900:CYN:N	2.51	0.73
2:M:433:ASP:OD1	2:M:437:LYS:HE2	1.89	0.73
2:O:425:ILE:O	2:O:426:ASN:CG	2.31	0.72
2:O:425:ILE:HD12	2:O:426:ASN:CA	2.18	0.72
2:O:425:ILE:C	2:O:426:ASN:CG	2.55	0.72
2:P:346:ARG:HH11	2:P:346:ARG:HB2	1.55	0.72
2:N:549:GLN:HG2	11:N:2291:HOH:O	1.89	0.72
2:N:424:ASN:H	2:N:424:ASN:HD22	1.38	0.72
2:O:356:VAL:HG23	2:O:361:ILE:HD11	1.71	0.72
2:O:657:PHE:CE1	2:O:658:ILE:CD1	2.70	0.72
2:O:352:LEU:CD2	2:O:484:LYS:HG3	2.19	0.72
1:C:260:GLN:NE2	11:C:785:HOH:O	2.23	0.71
2:O:352:LEU:HD13	2:O:481:ALA:HA	1.71	0.71
2:N:701:ASP:H	2:N:704:ILE:HG23	1.54	0.71
2:O:651:TYR:CE2	2:O:657:PHE:CD2	2.79	0.71
2:P:362:THR:H	2:P:464:GLN:NE2	1.88	0.70
2:P:491:ARG:O	2:P:495:LEU:HB2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:418:TRP:O	2:O:428:LEU:HA	1.91	0.70
2:P:423:ARG:HH21	2:P:488:ARG:NH1	1.88	0.70
2:M:451:LYS:NZ	2:M:454:GLU:OE2	2.25	0.70
2:O:396:GLN:HE22	2:O:398:ASP:HB2	1.56	0.70
2:P:424:ASN:HD22	2:P:424:ASN:N	1.90	0.70
2:O:399:PHE:CD2	2:O:399:PHE:O	2.44	0.70
2:M:408:HIS:HD2	2:M:419:HIS:ND1	1.90	0.70
2:P:356:VAL:O	2:P:391:TYR:HB2	1.91	0.70
1:B:535:ALA:HB3	1:B:537:ILE:HG12	1.74	0.70
2:M:150:ASP:OD2	2:M:152:THR:HG23	1.92	0.70
2:O:665:ALA:HB2	2:O:691:LEU:HD11	1.74	0.70
2:P:602:MET:HE1	2:P:645:MET:CE	2.21	0.70
1:D:614:ASP:N	6:D:963:GOL:H11	2.06	0.70
2:N:335:LYS:HD3	2:N:335:LYS:N	2.05	0.70
2:O:315:LYS:HD3	2:O:317:LYS:HE2	1.74	0.69
2:O:726:ASP:O	2:O:727:PRO:C	2.33	0.69
6:C:963:GOL:H12	2:O:27:HIS:CE1	2.28	0.69
2:N:369:ILE:HD12	2:N:466:THR:CG2	2.23	0.69
2:O:395:MET:CA	2:O:399:PHE:CZ	2.75	0.69
2:O:410:PHE:CD1	2:O:451:LYS:HD3	2.28	0.69
1:C:587:LYS:H	1:D:220:HIS:HE1	1.42	0.68
1:C:614:ASP:N	6:C:963:GOL:H11	2.08	0.68
1:D:515:ASN:HD22	1:D:518:THR:HG21	1.57	0.68
2:O:316:ILE:HG21	2:O:454:GLU:HG3	1.76	0.68
1:C:284:ASN:C	1:C:284:ASN:HD22	2.02	0.68
1:D:482:LEU:HD11	1:D:508:LEU:HD13	1.75	0.68
2:P:150:ASP:OD2	2:P:152:THR:HG22	1.94	0.68
1:B:114[B]:CYS:SG	1:B:208:ILE:HG21	2.34	0.68
2:O:418:TRP:HE3	2:O:429:ARG:HD2	1.59	0.68
2:O:423:ARG:HB3	2:O:424:ASN:HD22	1.58	0.68
2:O:445:GLY:O	2:O:449:VAL:HG23	1.94	0.68
1:A:284:ASN:HD22	1:A:286:LEU:H	1.42	0.67
2:M:704:ILE:HD11	2:M:711:ILE:HA	1.76	0.67
2:O:651:TYR:CD2	2:O:657:PHE:HD2	2.12	0.67
1:A:114[B]:CYS:SG	1:A:208:ILE:HG21	2.34	0.67
2:N:187:ASP:HA	2:N:211:ASN:HD22	1.58	0.67
2:O:658:ILE:O	2:O:658:ILE:HG22	1.95	0.67
2:P:500:VAL:O	2:P:553:LYS:NZ	2.23	0.67
2:O:485:TYR:HA	2:O:488:ARG:HE	1.58	0.67
2:N:150:ASP:OD2	2:N:152:THR:CG2	2.42	0.67
2:O:653:VAL:O	2:O:685:ARG:HD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:353:VAL:O	2:P:400:GLU:HG3	1.95	0.67
2:P:341:GLU:CD	2:P:427:TRP:HE1	2.03	0.67
2:O:157:ALA:HB3	2:O:183:LEU:CD2	2.25	0.67
2:O:524:ARG:O	2:O:524:ARG:HG3	1.94	0.66
2:P:602:MET:HE2	2:P:647:ILE:CG2	2.24	0.66
1:B:482:LEU:HD12	1:B:486:LYS:HE3	1.77	0.66
2:M:424:ASN:HD22	2:M:424:ASN:H	1.41	0.66
2:O:363:ASP:HB2	2:O:462:ARG:HD2	1.76	0.66
2:O:422:GLN:O	2:O:423:ARG:HB2	1.94	0.66
1:C:220:HIS:HE1	1:D:587:LYS:H	1.42	0.65
2:P:424:ASN:H	2:P:424:ASN:ND2	1.93	0.65
1:A:149[B]:ARG:NH2	1:A:250:ASP:OD2	2.29	0.65
1:B:370:ARG:HB3	11:B:1495:HOH:O	1.96	0.65
1:A:220:HIS:HD2	1:A:221:MET:O	1.80	0.65
2:O:490:ASP:C	2:O:493:ARG:HG2	2.21	0.65
2:P:246:ARG:HG2	2:P:246:ARG:HH11	1.60	0.65
1:A:105:MET:HE1	1:B:72:MET:HG2	1.70	0.65
2:O:482:ARG:CA	2:O:485:TYR:CE2	2.75	0.65
1:B:114[A]:CYS:SG	1:B:209:HIS:NE2	2.70	0.64
2:O:340:VAL:HG21	2:O:441:PHE:HZ	1.62	0.64
2:N:406:ARG:NH1	2:N:409:ASP:OD2	2.30	0.64
1:B:296:ARG:NH1	11:B:1789:HOH:O	2.31	0.64
1:A:220:HIS:HE1	1:B:587:LYS:H	1.46	0.64
2:O:420:THR:O	2:O:426:ASN:HA	1.98	0.64
2:O:424:ASN:HD22	2:O:424:ASN:N	1.96	0.64
2:O:604:ILE:HD12	2:O:606:PRO:HD3	1.79	0.63
2:O:551:ILE:HD13	2:O:567:VAL:HG23	1.81	0.63
1:A:299:GLU:O	1:A:303:LYS:HG2	1.98	0.62
2:O:376:ILE:HD12	2:O:382:LEU:CD2	2.29	0.62
2:O:478:MET:HE2	2:O:478:MET:O	2.00	0.62
2:P:402:VAL:HG21	2:P:538:ALA:HB2	1.82	0.62
2:P:483:GLU:O	2:P:487:GLU:CB	2.48	0.62
2:O:572:TYR:HD1	2:O:580:GLU:HB3	1.63	0.62
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.64	0.62
2:N:335:LYS:HD3	2:N:335:LYS:H	1.64	0.62
2:M:721:PRO:O	2:M:725:MET:HG3	2.00	0.62
1:A:209:HIS:HD2	1:B:213:SER:OG	1.83	0.62
2:P:537:LYS:HD3	2:P:541:GLU:OE2	1.99	0.61
1:D:414:SER:O	1:D:415:ASN:C	2.40	0.61
2:O:470:ASP:HB3	2:O:473:LYS:HB3	1.81	0.61
2:O:478:MET:CE	2:O:478:MET:CA	2.72	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:430:VAL:HG12	2:O:434:ALA:HB3	1.82	0.61
1:D:515:ASN:HD22	1:D:518:THR:CG2	2.13	0.61
2:O:352:LEU:HD21	2:O:484:LYS:HG3	1.81	0.61
2:O:424:ASN:C	2:O:425:ILE:HG23	2.25	0.61
2:P:341:GLU:OE2	2:P:346:ARG:NH1	2.34	0.60
2:O:144:PHE:O	2:O:148:MET:HG3	2.01	0.60
1:A:283:HIS:CD2	1:A:317:CYS:HB2	2.37	0.60
1:B:149:ARG:NH2	1:B:250:ASP:OD2	2.34	0.60
1:C:220:HIS:HD2	1:C:221:MET:O	1.84	0.60
2:O:727:PRO:O	2:O:729:MET:N	2.35	0.60
1:D:284:ASN:HD22	1:D:286:LEU:H	1.50	0.60
2:M:367:GLU:HG3	2:M:369:ILE:HD11	1.84	0.60
2:P:602:MET:CE	2:P:645:MET:HE3	2.31	0.60
2:N:150:ASP:OD2	2:N:152:THR:HG23	2.02	0.60
1:C:284:ASN:HD22	1:C:286:LEU:H	1.50	0.60
2:O:430:VAL:HG21	2:O:439:PHE:CE2	2.37	0.60
2:P:419:HIS:ND1	2:P:420:THR:N	2.49	0.60
2:P:572:TYR:CE2	2:P:577:ARG:HG2	2.37	0.60
2:O:341:GLU:CG	2:O:427:TRP:HE1	2.14	0.59
2:O:651:TYR:CD2	2:O:657:PHE:CE2	2.91	0.59
2:P:334:ARG:HG2	11:P:1790:HOH:O	2.03	0.59
1:D:68:CYS:HB2	1:D:97:ILE:HG23	1.85	0.59
2:N:354:ARG:CD	2:N:389:ASP:OD2	2.50	0.59
2:N:117[A]:ARG:HG3	11:N:2259:HOH:O	2.01	0.59
1:C:196[B]:GLU:OE2	2:O:120:LYS:NZ	2.36	0.59
2:O:435:VAL:C	2:O:437:LYS:H	2.10	0.59
2:P:483:GLU:O	2:P:487:GLU:HB2	2.03	0.59
1:D:195:LYS:O	1:D:199:ARG:HG3	2.03	0.59
1:D:466:LEU:HD22	1:D:595:TRP:HZ2	1.68	0.59
2:N:229:PHE:HD1	9:N:953:ACT:H2	1.66	0.59
1:B:305:ALA:CB	1:B:409:LYS:HE3	2.33	0.58
1:B:442:THR:HG21	1:B:535:ALA:HA	1.83	0.58
1:A:119:HIS:HE1	11:A:1427:HOH:O	1.85	0.58
2:M:245:ARG:HD3	11:M:918:HOH:O	2.02	0.58
2:N:595:CYS:HB2	9:N:953:ACT:H1	1.84	0.58
2:O:346:ARG:NH1	2:O:427:TRP:CE2	2.65	0.58
2:O:425:ILE:C	2:O:426:ASN:HD22	1.88	0.58
2:O:18:PRO:HD2	2:O:22:PHE:CZ	2.38	0.58
2:O:425:ILE:O	2:O:426:ASN:HB3	2.01	0.58
2:P:187:ASP:HA	2:P:211:ASN:HD22	1.66	0.58
1:B:114[A]:CYS:SG	1:B:209:HIS:CD2	2.97	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:491:ARG:O	2:O:495:LEU:HB2	2.03	0.58
2:O:371:PRO:HD2	2:O:469:THR:HB	1.84	0.58
2:P:361:ILE:HG21	2:P:462:ARG:HD3	1.85	0.58
1:A:587:LYS:H	1:B:220:HIS:HE1	1.52	0.57
1:B:283:HIS:CD2	1:B:317:CYS:HB2	2.39	0.57
2:O:324:PHE:CE2	2:O:451:LYS:HE2	2.39	0.57
1:D:614:ASP:H	6:D:963:GOL:H11	1.68	0.57
2:O:346:ARG:HG3	2:O:381:LYS:NZ	2.19	0.57
2:O:394:LYS:HG2	2:O:395:MET:H	1.68	0.57
2:O:658:ILE:CG2	2:O:661:ASP:HB2	2.33	0.57
1:A:114[B]:CYS:SG	1:A:208:ILE:CG2	2.93	0.57
1:C:209:HIS:HD2	1:D:213:SER:OG	1.87	0.57
2:O:352:LEU:HD22	2:O:484:LYS:HG3	1.84	0.57
2:M:602:MET:CE	2:M:647:ILE:HD13	2.34	0.57
2:O:722:ALA:HA	2:O:725:MET:SD	2.44	0.57
2:P:583:CYS:HB2	2:P:586:THR:HG22	1.87	0.57
2:O:64:VAL:HB	2:O:223:LEU:HD12	1.87	0.57
1:A:426:ARG:HH21	1:A:539:ILE:HD12	1.70	0.57
2:N:23:ARG:NH1	11:N:855:HOH:O	2.36	0.57
2:N:588:MET:HE2	2:N:729:MET:O	2.03	0.57
2:O:424:ASN:N	2:O:424:ASN:ND2	2.50	0.57
2:P:402:VAL:HG21	2:P:538:ALA:CB	2.35	0.57
2:O:316:ILE:HG23	2:O:454:GLU:HG3	1.86	0.57
2:P:399:PHE:HE2	2:P:541:GLU:HG3	1.70	0.56
1:A:577:VAL:HG11	1:A:645:ILE:HG23	1.88	0.56
1:C:186:LEU:CD2	1:C:205:PRO:HD2	2.35	0.56
1:C:283:HIS:CD2	1:C:317:CYS:HB2	2.40	0.56
2:O:666:ARG:CZ	2:O:725:MET:HE2	2.35	0.56
2:M:314:THR:O	2:M:315:LYS:C	2.49	0.56
2:O:356:VAL:HG23	2:O:361:ILE:CD1	2.36	0.56
1:B:24:ASN:O	1:B:27:ARG:HG2	2.06	0.56
1:B:482:LEU:CD1	1:B:486:LYS:HE3	2.35	0.55
2:M:383:PRO:HG3	2:M:471:GLU:HG3	1.87	0.55
2:P:419:HIS:ND1	2:P:419:HIS:C	2.64	0.55
2:P:457:PRO:O	2:P:458:ALA:CB	2.54	0.55
1:B:447:ASN:HD22	1:B:450:ARG:HB2	1.72	0.55
2:N:150:ASP:OD2	2:N:152:THR:HG22	2.06	0.55
2:O:613:ILE:HD12	2:O:670:MET:HE3	1.88	0.55
1:A:426:ARG:CZ	11:A:2027:HOH:O	2.54	0.55
2:N:335:LYS:H	2:N:335:LYS:CD	2.19	0.55
1:C:460:GLU:CD	1:C:530:ARG:HH22	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:ARG:NH1	11:D:2194:HOH:O	2.38	0.55
1:D:220:HIS:HD2	1:D:221:MET:O	1.90	0.55
2:M:354:ARG:HD2	2:M:389:ASP:OD2	2.07	0.55
2:O:418:TRP:O	2:O:428:LEU:HD13	2.06	0.55
2:M:163:ALA:HB2	2:M:169:LEU:HG	1.89	0.54
1:A:112:ALA:HA	1:B:217:ASN:HD22	1.72	0.54
1:B:537:ILE:CG2	1:B:540:GLY:H	2.20	0.54
2:P:150:ASP:OD2	2:P:152:THR:CG2	2.54	0.54
1:A:368:HIS:NE2	1:A:416:ARG:HG3	2.23	0.54
1:A:122:HIS:HD2	11:A:926:HOH:O	1.90	0.54
1:B:601:PRO:HD3	1:B:652:ARG:CZ	2.36	0.54
2:O:480:VAL:O	2:O:484:LYS:HB2	2.07	0.54
2:N:369:ILE:HD12	2:N:466:THR:HG21	1.89	0.54
2:O:447:ILE:O	2:O:451:LYS:HB2	2.07	0.54
1:C:284:ASN:ND2	1:C:286:LEU:H	2.06	0.54
2:P:420:THR:CG2	2:P:420:THR:O	2.55	0.54
2:N:408:HIS:HD2	2:N:419:HIS:ND1	2.06	0.54
2:O:479:GLU:O	2:O:483:GLU:HG3	2.07	0.54
1:A:119:HIS:CE1	11:A:1427:HOH:O	2.60	0.54
2:O:388:VAL:HG13	2:O:465:VAL:HG22	1.88	0.54
2:P:335:LYS:H	2:P:335:LYS:HD2	1.72	0.54
2:N:66:ARG:HD3	11:N:754:HOH:O	2.07	0.53
1:C:187:MET:HE3	1:C:195:LYS:HG2	1.90	0.53
2:O:157:ALA:HB3	2:O:183:LEU:HD23	1.91	0.53
2:O:609:ASN:ND2	2:O:725:MET:O	2.41	0.53
2:O:684:ARG:NH1	2:O:685:ARG:HG2	2.23	0.53
1:B:114[B]:CYS:SG	1:B:208:ILE:CG2	2.96	0.53
2:O:324:PHE:CZ	2:O:451:LYS:HE2	2.43	0.53
1:D:470:CYS:O	1:D:582:GLU:HB2	2.09	0.53
1:D:260:GLN:NE2	11:D:1371:HOH:O	2.41	0.53
2:O:416:GLY:O	2:O:430:VAL:HA	2.09	0.53
2:P:387:LEU:O	2:P:465:VAL:HA	2.09	0.53
2:P:457:PRO:O	2:P:458:ALA:HB2	2.08	0.53
1:D:460:GLU:OE1	1:D:530:ARG:NH2	2.42	0.53
2:O:423:ARG:C	2:O:424:ASN:ND2	2.67	0.53
1:A:114[A]:CYS:SG	1:A:209:HIS:NE2	2.82	0.53
1:C:149:ARG:HD3	11:C:1313:HOH:O	2.09	0.53
1:A:284:ASN:ND2	1:A:286:LEU:H	2.06	0.53
1:D:601:PRO:HD3	1:D:652:ARG:CZ	2.39	0.53
2:P:300:LYS:NZ	11:P:1581:HOH:O	2.34	0.53
1:D:550:CYS:HB3	5:D:900:CYN:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ARG:NH2	1:D:250:ASP:OD2	2.38	0.52
2:N:349:ALA:HA	2:N:384:LEU:O	2.10	0.52
2:N:618:HIS:CE1	2:N:702:GLU:HG2	2.43	0.52
2:N:681:GLU:HG2	2:N:684:ARG:HH21	1.75	0.52
2:O:621:MET:HE1	2:O:625:GLY:HA2	1.90	0.52
2:P:354:ARG:CD	2:P:356:VAL:HG13	2.31	0.52
1:B:284:ASN:HD22	1:B:286:LEU:H	1.56	0.52
2:N:602:MET:HE3	2:N:611:ILE:CD1	2.40	0.52
1:C:114:CYS:SG	1:C:209:HIS:NE2	2.83	0.52
2:N:199:LYS:HE3	2:N:204:TYR:OH	2.09	0.52
2:O:503:PHE:O	2:O:551:ILE:N	2.28	0.52
2:M:173:VAL:O	2:M:177:MET:HG3	2.10	0.52
2:O:421:GLY:HA3	2:O:425:ILE:HD11	1.91	0.52
2:P:239:GLU:HG2	11:P:2373:HOH:O	2.08	0.52
2:O:651:TYR:O	2:O:657:PHE:CD2	2.63	0.52
2:P:399:PHE:CE2	2:P:541:GLU:HG3	2.44	0.52
1:D:284:ASN:HD22	1:D:284:ASN:C	2.18	0.52
1:A:284:ASN:HD22	1:A:284:ASN:C	2.17	0.51
2:O:346:ARG:HG3	2:O:381:LYS:HZ3	1.74	0.51
2:O:80:PRO:HB2	2:O:81:PRO:HD3	1.92	0.51
1:A:201:HIS:HE1	2:M:35:TYR:OH	1.94	0.51
1:C:186:LEU:HD22	1:C:205:PRO:HD2	1.92	0.51
2:O:341:GLU:CD	2:O:427:TRP:HE1	2.18	0.51
2:P:174:LYS:HE2	2:P:175:GLU:N	2.26	0.51
1:C:81[B]:THR:HG23	1:C:82:ASP:OD2	2.09	0.51
2:M:150:ASP:OD2	2:M:152:THR:CG2	2.57	0.51
2:O:668:VAL:HG12	2:O:720:HIS:CE1	2.46	0.51
2:P:602:MET:CE	2:P:645:MET:CE	2.89	0.51
1:A:213:SER:OG	1:B:209:HIS:HD2	1.94	0.51
2:M:339:TYR:HD2	2:M:340:VAL:HG22	1.75	0.51
2:O:712:LEU:HB3	2:O:713:PRO:HD3	1.91	0.51
2:P:61:TYR:HD1	2:P:66:ARG:HD2	1.76	0.51
1:C:486:LYS:HE2	1:C:519:TYR:CE2	2.46	0.51
2:O:590:ASN:N	2:O:591:PRO:HD3	2.25	0.51
2:P:341:GLU:CD	2:P:427:TRP:NE1	2.69	0.51
1:B:470:CYS:O	1:B:582:GLU:HB2	2.11	0.51
2:O:658:ILE:HG23	2:O:661:ASP:HB2	1.93	0.51
1:A:200:THR:OG1	1:A:201:HIS:HD2	1.94	0.50
1:D:317:CYS:O	1:D:321:GLU:HG2	2.11	0.50
2:P:505:SER:HB3	2:P:570:TYR:CE2	2.46	0.50
2:M:2:THR:N	11:M:2199:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:423:ARG:C	2:O:424:ASN:HD22	2.19	0.50
1:C:20:MET:HE1	1:C:479:ASN:HD22	1.77	0.50
2:M:328:PHE:O	2:M:331:GLU:HB2	2.11	0.50
6:A:963:GOL:H11	2:M:27:HIS:CE1	2.47	0.50
2:N:300:LYS:HD2	11:N:1484:HOH:O	2.11	0.50
2:N:640:GLN:HA	11:N:954:HOH:O	2.10	0.50
2:P:339:TYR:CE1	2:P:435:VAL:HG11	2.47	0.50
2:O:397:ALA:HA	2:O:400:GLU:OE1	2.12	0.49
2:O:425:ILE:N	2:O:426:ASN:ND2	2.59	0.49
2:P:124:ASP:OD1	2:P:125:GLU:OE1	2.29	0.49
2:P:602:MET:CE	2:P:647:ILE:HG21	2.36	0.49
1:A:515:ASN:ND2	1:A:518:THR:HG21	2.23	0.49
1:B:201:HIS:HE1	2:N:35:TYR:OH	1.95	0.49
1:C:615:LEU:C	1:C:615:LEU:HD23	2.37	0.49
1:D:370:ARG:HD2	1:D:384:TYR:CE2	2.47	0.49
2:N:618:HIS:HE1	2:N:702:GLU:HG2	1.76	0.49
2:O:456:PHE:N	2:O:457:PRO:HD3	2.27	0.49
2:O:657:PHE:O	2:O:663:GLY:HA2	2.12	0.49
2:P:420:THR:O	2:P:420:THR:HG23	2.12	0.49
1:A:220:HIS:CD2	1:A:221:MET:O	2.62	0.49
1:D:114:CYS:SG	1:D:209:HIS:NE2	2.86	0.49
2:O:609:ASN:HB3	2:O:722:ALA:O	2.12	0.49
1:B:394:ILE:HG23	1:B:395:GLU:N	2.28	0.49
2:M:86:LYS:NZ	11:M:2207:HOH:O	2.45	0.49
2:M:602:MET:CE	2:M:647:ILE:HG21	2.34	0.49
2:O:479:GLU:HA	2:O:482:ARG:HB2	1.95	0.49
2:O:522:PRO:HD3	2:O:533:TRP:CD1	2.48	0.49
1:C:577:VAL:HG11	1:C:645:ILE:HG23	1.95	0.49
2:O:602:MET:SD	2:O:658:ILE:HD11	2.53	0.49
2:O:670:MET:HE2	2:O:674:LEU:HG	1.94	0.49
1:B:305:ALA:HB1	1:B:409:LYS:HE3	1.95	0.49
1:A:112:ALA:HA	1:B:217:ASN:ND2	2.28	0.49
2:O:411:ILE:HD13	2:O:428:LEU:HD11	1.93	0.49
2:O:443:ASN:HA	2:O:446:GLU:OE2	2.12	0.49
2:P:351:GLU:OE2	2:P:426:ASN:ND2	2.46	0.49
2:P:481:ALA:HB1	2:P:485:TYR:CZ	2.48	0.49
2:M:169:LEU:HD13	2:M:193:LEU:HG	1.95	0.49
2:O:372:ASP:CG	2:O:440:ARG:HG3	2.38	0.49
2:O:399:PHE:CD2	2:O:399:PHE:C	2.90	0.49
2:P:585:TYR:CE2	2:P:656:LYS:HD2	2.47	0.49
1:D:201:HIS:HE1	1:D:627:VAL:HG13	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:61:TYR:HD1	2:N:66:ARG:HD2	1.78	0.48
2:N:374:ASP:HB3	2:N:440:ARG:HH21	1.77	0.48
2:O:63:PRO:HB2	2:O:220:ASN:HB2	1.96	0.48
2:O:71:GLU:HG3	2:O:82:ILE:CD1	2.38	0.48
2:O:651:TYR:CE2	2:O:657:PHE:HD2	2.28	0.48
2:M:568:ASN:HD21	2:M:581:GLN:HE21	1.61	0.48
1:D:316:CYS:H	1:D:503:GLN:HE22	1.61	0.48
1:D:615:LEU:H	6:D:963:GOL:C1	2.25	0.48
2:N:350:PHE:CD1	2:N:350:PHE:C	2.92	0.48
2:O:396:GLN:NE2	2:O:398:ASP:HB2	2.25	0.48
1:A:550:CYS:HB3	5:A:900:CYN:N	2.29	0.48
2:N:246:ARG:C	2:N:247:ARG:HD2	2.38	0.48
2:M:187:ASP:HA	2:M:211:ASN:HD22	1.78	0.48
2:M:540:TYR:O	2:M:544:HIS:HD2	1.96	0.48
2:M:424:ASN:HD22	2:M:424:ASN:N	2.07	0.48
2:N:315:LYS:H	2:N:315:LYS:HD2	1.77	0.48
2:O:597:CYS:HB3	9:O:953:ACT:H1	1.96	0.48
1:A:104[A]:LEU:CD2	1:B:104[A]:LEU:HD22	2.43	0.48
1:A:201:HIS:CE1	2:M:35:TYR:OH	2.67	0.48
1:C:79:LYS:NZ	11:C:2087:HOH:O	2.38	0.48
1:D:201:HIS:CE1	2:P:35:TYR:OH	2.67	0.48
2:O:289:PRO:O	2:O:290:ASP:HB2	2.12	0.48
2:O:725:MET:O	2:O:726:ASP:C	2.56	0.48
1:C:278:PHE:HB3	1:C:312:LEU:HD23	1.96	0.48
2:O:589:GLU:C	2:O:591:PRO:HD3	2.38	0.48
2:P:163:ALA:CB	2:P:169:LEU:HB2	2.44	0.48
2:P:602:MET:HE2	2:P:647:ILE:HD13	1.96	0.48
1:D:280:LEU:HD13	1:D:288:SER:HB2	1.95	0.48
2:O:372:ASP:O	2:O:376:ILE:HG12	2.13	0.48
1:B:284:ASN:HD22	1:B:284:ASN:C	2.21	0.47
1:D:186:LEU:CD2	1:D:205:PRO:HD2	2.44	0.47
2:O:350:PHE:CD1	2:O:481:ALA:HB2	2.49	0.47
1:A:284:ASN:HD21	1:A:286:LEU:HG	1.80	0.47
1:D:215:LEU:HD22	1:D:234:ALA:HA	1.96	0.47
2:N:492:MET:HE2	11:N:1937:HOH:O	2.14	0.47
2:O:243:TYR:CE2	2:O:247:ARG:HD2	2.49	0.47
1:A:104[A]:LEU:HD22	1:B:104[A]:LEU:CD2	2.45	0.47
1:C:201:HIS:HE1	2:O:35:TYR:OH	1.97	0.47
2:O:389:ASP:HB2	2:O:464:GLN:HB3	1.95	0.47
1:C:149:ARG:NH2	1:C:250:ASP:OD2	2.46	0.47
2:O:698:LYS:HA	2:O:718:LYS:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:515:ASN:ND2	1:D:518:THR:HG21	2.25	0.47
2:O:469:THR:O	2:O:470:ASP:HB2	2.15	0.47
2:O:470:ASP:O	2:O:474:VAL:HG22	2.14	0.47
2:O:230:GLY:HA3	2:O:243:TYR:CE2	2.50	0.47
2:P:611:ILE:HD11	2:P:667:ILE:HG12	1.96	0.47
2:O:2:THR:HA	2:O:5:ASP:OD1	2.14	0.47
1:A:149[A]:ARG:NH2	1:A:250:ASP:OD2	2.44	0.47
1:A:482:LEU:CD1	1:A:486:LYS:HE3	2.45	0.47
2:O:79:LEU:N	2:O:80:PRO:CD	2.78	0.47
2:P:701:ASP:H	2:P:704:ILE:HD13	1.80	0.47
2:P:555:GLY:HA3	2:P:565:LYS:HB3	1.97	0.47
2:P:668:VAL:HB	2:P:715:LEU:HD11	1.97	0.46
1:B:267:ASN:O	1:B:270:VAL:HG22	2.15	0.46
6:D:963:GOL:H12	2:P:27:HIS:CE1	2.50	0.46
2:M:657:PHE:O	2:M:663:GLY:HA2	2.15	0.46
2:O:113:ILE:O	2:O:117[A]:ARG:HG3	2.15	0.46
2:P:351:GLU:HG2	2:P:426:ASN:OD1	2.16	0.46
2:O:376:ILE:HD13	2:O:382:LEU:HD21	1.97	0.46
1:A:217:ASN:HD22	1:B:112:ALA:HA	1.80	0.46
2:M:426:ASN:C	2:M:426:ASN:HD22	2.23	0.46
2:N:160:LEU:HD13	2:N:215:ILE:HD13	1.97	0.46
2:O:157:ALA:HB3	2:O:183:LEU:HD22	1.98	0.46
2:P:444:TYR:O	2:P:448:LEU:HD22	2.16	0.46
1:A:482:LEU:HD13	1:A:486:LYS:HE3	1.97	0.46
1:D:283:HIS:CD2	1:D:317:CYS:HB2	2.51	0.46
2:M:339:TYR:CG	2:M:435:VAL:HG21	2.49	0.46
1:A:483:THR:HB	1:A:638:PRO:HB2	1.97	0.46
1:B:661[A]:GLU:HG3	1:B:665:ARG:HH21	1.81	0.46
2:N:604:ILE:HG13	2:N:643:GLY:O	2.16	0.46
2:O:439:PHE:CE1	2:O:443:ASN:HB2	2.51	0.46
2:O:602:MET:HE1	2:O:645:MET:HE2	1.97	0.46
2:P:384:LEU:HA	2:P:468:PHE:O	2.16	0.46
2:O:122:LYS:HB2	2:O:125:GLU:HG3	1.97	0.46
1:B:367:TYR:HA	1:B:416:ARG:HH12	1.81	0.46
1:C:118:ASN:OD1	1:C:209:HIS:HE1	1.99	0.46
1:D:201:HIS:CE1	1:D:627:VAL:HG13	2.50	0.46
2:O:566:SER:HB3	11:O:1472:HOH:O	2.16	0.46
1:D:31:PRO:HB2	1:D:423:ILE:HD13	1.98	0.46
1:D:201:HIS:HE1	2:P:35:TYR:OH	1.99	0.46
1:C:114:CYS:SG	1:C:209:HIS:CD2	3.09	0.45
1:C:626:ASP:HB3	2:O:212:PHE:CG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:674:LEU:HD22	2:N:678:LEU:HG	1.98	0.45
2:M:347:THR:CG2	2:M:381:LYS:HG3	2.47	0.45
2:O:399:PHE:CZ	2:O:459:ILE:HD13	2.51	0.45
2:O:481:ALA:O	2:O:485:TYR:HD2	1.90	0.45
1:B:201:HIS:CE1	2:N:35:TYR:OH	2.70	0.45
1:C:220:HIS:CD2	1:C:221:MET:O	2.67	0.45
2:O:339:TYR:HB3	2:O:373:ILE:HD11	1.99	0.45
2:O:603:ALA:HB3	2:O:612:MET:HG3	1.99	0.45
2:P:338:MET:HG2	2:P:339:TYR:H	1.81	0.45
1:B:537:ILE:HG22	1:B:540:GLY:H	1.81	0.45
1:B:539:ILE:HD13	1:B:539:ILE:H	1.81	0.45
1:C:614:ASP:H	6:C:963:GOL:H32	1.81	0.45
2:P:389:ASP:HB2	2:P:464:GLN:HG3	1.99	0.45
2:P:483:GLU:O	2:P:487:GLU:HB3	2.15	0.45
1:A:209:HIS:HD2	1:B:213:SER:CB	2.30	0.45
1:B:118:ASN:C	1:B:118:ASN:HD22	2.25	0.45
2:N:342:MET:SD	2:N:342:MET:N	2.90	0.45
2:O:470:ASP:HB3	2:O:473:LYS:CB	2.47	0.45
1:D:466:LEU:CD2	1:D:595:TRP:CZ2	2.97	0.45
2:M:657:PHE:O	2:M:658:ILE:C	2.60	0.45
2:O:505:SER:HB3	2:O:570:TYR:HE2	1.82	0.45
2:P:391:TYR:HB3	2:P:462:ARG:HH11	1.72	0.45
1:B:114[B]:CYS:CB	1:B:208:ILE:HG21	2.47	0.45
1:B:573:LYS:HE2	1:B:671:CYS:O	2.17	0.45
2:M:23:ARG:NH1	11:M:1046:HOH:O	2.20	0.45
2:O:652:ILE:HA	2:O:657:PHE:CE2	2.52	0.45
2:N:613:ILE:O	2:N:671:PRO:HD3	2.17	0.44
2:P:391:TYR:HB3	2:P:462:ARG:HH12	1.76	0.44
2:P:589:GLU:O	2:P:590:ASN:C	2.60	0.44
1:B:114[B]:CYS:HB3	1:B:208:ILE:HG21	1.98	0.44
2:M:247:ARG:HD2	2:M:247:ARG:HA	1.52	0.44
2:N:602:MET:HE1	2:N:658:ILE:HG21	2.00	0.44
2:O:419:HIS:HE1	2:O:421:GLY:O	2.01	0.44
2:O:515:ASN:O	2:O:575:SER:HB2	2.17	0.44
2:O:727:PRO:O	2:O:728:ILE:C	2.60	0.44
2:P:246:ARG:HG2	2:P:246:ARG:NH1	2.30	0.44
2:P:576:ASN:O	2:P:577:ARG:HB2	2.17	0.44
1:A:315:ILE:HG12	1:A:331:VAL:CG1	2.47	0.44
2:N:16:LYS:HE2	2:N:16:LYS:HB3	1.75	0.44
2:O:505:SER:HB3	2:O:570:TYR:CE2	2.52	0.44
1:C:587:LYS:HB3	5:C:900:CYN:C	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:CYS:HB2	1:D:97:ILE:CG2	2.46	0.44
2:O:344:GLY:O	2:O:346:ARG:HD3	2.18	0.44
1:A:331:VAL:HG13	1:A:332:THR:N	2.32	0.44
2:N:604:ILE:HG13	2:N:604:ILE:H	1.63	0.44
2:O:169:LEU:CD1	2:O:193:LEU:HG	2.47	0.44
2:O:482:ARG:HA	2:O:485:TYR:HE2	1.69	0.44
2:O:598:PHE:CE1	2:O:601:ILE:HD11	2.53	0.44
2:P:113:ILE:O	2:P:117[A]:ARG:HG3	2.17	0.44
2:M:481:ALA:HB1	2:M:485:TYR:CZ	2.53	0.44
2:N:579:LEU:HD11	2:N:593:THR:HG21	1.99	0.44
2:P:453:LYS:HG3	2:P:463:VAL:CG2	2.47	0.44
2:P:459:ILE:HD13	2:P:542:ILE:HB	2.00	0.44
2:P:626:MET:HB2	2:P:631:LEU:HD22	1.99	0.44
1:C:213:SER:OG	1:D:209:HIS:HD2	2.00	0.44
1:D:293:GLN:NE2	1:D:296:ARG:HH11	2.16	0.44
6:D:963:GOL:H2	2:P:27:HIS:HE1	1.83	0.44
2:M:408:HIS:CD2	2:M:419:HIS:ND1	2.78	0.44
2:N:315:LYS:O	2:N:316:ILE:C	2.61	0.44
2:N:683:VAL:HG13	2:N:693:GLU:HG3	2.00	0.44
2:O:169:LEU:HD13	2:O:193:LEU:HD21	2.00	0.44
2:P:460:VAL:CG1	2:P:463:VAL:HG22	2.47	0.44
2:P:595:CYS:HB2	9:P:953:ACT:H1	1.98	0.44
2:P:721:PRO:O	2:P:725:MET:HG3	2.18	0.44
1:D:114:CYS:CA	11:D:1014:HOH:O	2.66	0.44
1:D:284:ASN:HD21	1:D:286:LEU:HG	1.83	0.44
2:M:320:LEU:HB3	2:M:321:PRO:HD2	2.00	0.44
2:N:602:MET:HE3	2:N:611:ILE:HD13	2.00	0.43
2:O:340:VAL:HG22	2:O:373:ILE:HD12	2.00	0.43
2:O:425:ILE:HD12	2:O:425:ILE:O	2.02	0.43
2:O:425:ILE:HD12	2:O:426:ASN:HA	1.98	0.43
2:O:484:LYS:HD3	2:O:484:LYS:HA	1.64	0.43
2:O:715:LEU:HD22	2:O:720:HIS:CD2	2.53	0.43
2:P:340:VAL:HG21	2:P:376:ILE:HD11	2.00	0.43
2:P:553:LYS:HG2	2:P:564:TRP:NE1	2.33	0.43
2:M:670:MET:HE3	2:M:674:LEU:HB3	2.00	0.43
2:O:425:ILE:CA	2:O:426:ASN:ND2	2.80	0.43
2:O:657:PHE:CZ	2:O:658:ILE:CD1	3.01	0.43
2:P:339:TYR:CE1	2:P:378:GLU:HG3	2.52	0.43
1:C:190:ILE:HG13	1:C:195:LYS:HG3	2.00	0.43
1:D:118:ASN:C	1:D:118:ASN:HD22	2.27	0.43
2:M:366:ILE:HA	2:M:465:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:339:TYR:CG	2:N:435:VAL:HG21	2.54	0.43
2:O:657:PHE:C	2:O:659:SER:N	2.72	0.43
2:O:658:ILE:HG22	2:O:661:ASP:HB2	2.00	0.43
2:P:489:ASP:O	2:P:493:ARG:HB2	2.17	0.43
2:O:395:MET:HB3	2:O:396:GLN:H	1.56	0.43
2:O:423:ARG:CB	2:O:424:ASN:HD22	2.27	0.43
2:O:557:ILE:HD11	2:O:565:LYS:HB2	1.99	0.43
2:O:626:MET:HB2	2:O:631:LEU:HD13	1.99	0.43
1:C:114:CYS:CA	11:C:1383:HOH:O	2.66	0.43
2:O:71:GLU:H	2:O:71:GLU:CD	2.21	0.43
2:O:658:ILE:O	2:O:658:ILE:CG2	2.65	0.43
2:P:423:ARG:HH21	2:P:488:ARG:HH12	1.66	0.43
1:B:200:THR:OG1	1:B:201:HIS:HD2	2.00	0.43
6:D:963:GOL:H2	2:P:27:HIS:CE1	2.54	0.43
2:O:602:MET:HE1	2:O:645:MET:CE	2.48	0.43
2:P:565:LYS:O	2:P:565:LYS:HD3	2.19	0.43
1:A:118:ASN:OD1	1:A:209:HIS:HE1	2.01	0.43
1:C:284:ASN:HD22	1:C:285:PRO:N	2.17	0.43
1:D:114:CYS:SG	1:D:209:HIS:CD2	3.12	0.43
2:P:400:GLU:OE2	2:P:484:LYS:HE2	2.13	0.43
2:O:383:PRO:HB2	2:O:474:VAL:HG21	2.01	0.43
1:A:278:PHE:HB3	1:A:312:LEU:HD23	2.00	0.43
1:A:550:CYS:CB	5:A:900:CYN:N	2.82	0.43
1:C:176:ARG:O	1:C:207:GLY:HA3	2.19	0.43
2:M:164:LYS:HD3	2:M:298:TYR:CE1	2.54	0.43
2:P:272:THR:HG22	2:P:272:THR:O	2.19	0.43
2:P:342:MET:CG	2:P:384:LEU:HD22	2.40	0.43
2:P:400:GLU:OE1	2:P:484:LYS:HE3	2.18	0.43
1:B:220:HIS:HD2	1:B:221:MET:O	2.01	0.42
2:M:640[A]:GLN:HA	11:M:906:HOH:O	2.19	0.42
2:O:353:VAL:HG22	2:O:388:VAL:HB	2.00	0.42
2:O:393:ARG:HG3	2:O:394:LYS:N	2.31	0.42
2:O:532:SER:H	2:O:535:ASP:HB2	1.84	0.42
2:O:669:TRP:HA	2:O:700:ALA:O	2.19	0.42
2:P:471:GLU:HA	2:P:474:VAL:HG12	2.01	0.42
1:B:515:ASN:HA	1:B:518:THR:HG23	2.01	0.42
1:C:442:THR:HG21	1:C:537:ILE:HD11	2.00	0.42
2:M:61:TYR:HD1	2:M:66:ARG:HD2	1.84	0.42
2:N:247:ARG:HD2	2:N:247:ARG:HA	1.82	0.42
2:O:435:VAL:C	2:O:437:LYS:N	2.77	0.42
2:O:572:TYR:HA	2:O:579:LEU:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:602:MET:HE2	2:O:647:ILE:HG12	2.01	0.42
2:P:448:LEU:O	2:P:452:MET:HG2	2.18	0.42
2:P:541:GLU:H	2:P:541:GLU:HG2	1.63	0.42
1:A:217:ASN:ND2	1:B:112:ALA:HA	2.33	0.42
1:C:615:LEU:HD23	1:C:615:LEU:O	2.19	0.42
2:O:365:LYS:C	2:O:366:ILE:HG13	2.44	0.42
2:P:486:LYS:H	2:P:486:LYS:HG2	1.71	0.42
1:B:122:HIS:HD2	11:B:925:HOH:O	2.03	0.42
1:B:190:ILE:HG13	1:B:195:LYS:HG3	2.01	0.42
1:B:299:GLU:O	1:B:303:LYS:HG3	2.19	0.42
1:C:298:MET:HE3	1:C:298:MET:HB3	1.98	0.42
2:M:702:GLU:H	2:M:702:GLU:HG3	1.31	0.42
2:N:384:LEU:HA	2:N:468:PHE:O	2.19	0.42
2:O:692:GLY:C	2:O:694:ASP:H	2.26	0.42
2:N:500:VAL:O	2:N:553:LYS:NZ	2.42	0.42
2:M:272:THR:HG22	2:M:272:THR:O	2.19	0.42
2:N:64:VAL:HG23	2:N:220:ASN:HB3	2.01	0.42
2:O:3:ASP:O	2:O:6:LYS:HG2	2.20	0.42
2:P:287:GLN:NE2	2:P:289:PRO:HD3	2.34	0.42
1:B:238:ALA:O	1:B:241:ASP:HB3	2.20	0.42
1:D:208:ILE:HG21	11:D:1014:HOH:O	2.19	0.42
2:M:339:TYR:HD2	2:M:340:VAL:CG2	2.32	0.42
2:P:7:ILE:HD13	2:P:245:ARG:HG3	2.02	0.42
1:B:217:ASN:O	1:B:223:MET:HG3	2.19	0.42
1:C:98:VAL:HG13	1:C:610:VAL:HA	2.02	0.42
2:N:247:ARG:HD2	2:N:247:ARG:N	2.32	0.42
2:O:439:PHE:O	2:O:440:ARG:HD3	2.20	0.42
1:A:394:ILE:HG23	1:A:395:GLU:N	2.35	0.42
1:D:28:THR:OG1	1:D:477:GLN:NE2	2.53	0.42
1:D:128:ALA:HA	1:D:160:LEU:HD22	2.02	0.42
1:D:307:ALA:HB2	1:D:408:PHE:CE2	2.54	0.42
1:B:571:THR:N	1:B:572:PRO:CD	2.83	0.42
2:N:353:VAL:HG22	2:N:388:VAL:HB	2.01	0.42
2:O:352:LEU:CD1	2:O:481:ALA:HA	2.47	0.42
1:D:339:LEU:HD13	1:D:339:LEU:HA	1.87	0.41
2:O:7:ILE:HD13	2:O:245:ARG:HD2	2.00	0.41
2:O:411:ILE:HG21	2:O:428:LEU:CD1	2.50	0.41
1:D:414:SER:O	1:D:415:ASN:O	2.39	0.41
2:M:384:LEU:HD11	2:M:467:ILE:HG23	2.01	0.41
2:O:266:ALA:HB1	2:O:276:VAL:HG21	2.01	0.41
2:O:307:GLU:HG3	2:O:308:THR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:423:ARG:HH21	2:P:488:ARG:HH11	1.62	0.41
2:P:583:CYS:SG	2:P:589:GLU:HG2	2.60	0.41
2:M:179:MET:HE3	2:M:179:MET:HB2	1.90	0.41
2:N:262:LYS:HG3	11:N:2270:HOH:O	2.20	0.41
2:N:439:PHE:CE1	2:N:443:ASN:HB2	2.55	0.41
2:O:347:THR:HA	2:O:348:PRO:HD2	1.82	0.41
2:O:395:MET:O	2:O:396:GLN:CB	2.67	0.41
2:O:431:SER:OG	2:O:434:ALA:HB2	2.20	0.41
2:O:613:ILE:O	2:O:671:PRO:HD3	2.20	0.41
2:O:720:HIS:HA	2:O:721:PRO:HD3	1.84	0.41
2:O:728:ILE:O	2:O:729:MET:C	2.63	0.41
1:A:529:LYS:HE2	11:A:1060:HOH:O	2.20	0.41
1:B:284:ASN:ND2	1:B:286:LEU:H	2.18	0.41
1:C:384:TYR:CE2	2:P:88:ALA:HB2	2.56	0.41
2:O:534:LEU:HD12	2:O:534:LEU:N	2.36	0.41
2:P:382:LEU:HG	2:P:469:THR:HB	2.02	0.41
1:B:374:THR:HA	1:B:386:ILE:O	2.21	0.41
1:B:394:ILE:HG23	1:B:395:GLU:H	1.85	0.41
1:C:601:PRO:HD3	1:C:652:ARG:CZ	2.51	0.41
1:D:510:LEU:O	1:D:543:PRO:HD2	2.20	0.41
2:M:568:ASN:ND2	2:M:581:GLN:HE21	2.19	0.41
2:O:505:SER:CB	2:O:570:TYR:HE2	2.33	0.41
2:P:169:LEU:HG	2:P:193:LEU:HD21	2.02	0.41
1:A:241:ASP:OD2	1:A:241:ASP:C	2.63	0.41
2:M:602:MET:CE	2:M:657:PHE:CE2	2.91	0.41
2:P:390:ILE:HD13	2:P:463:VAL:HG13	2.02	0.41
1:B:298:MET:HE1	1:B:402:ARG:HG3	2.02	0.41
1:B:447:ASN:ND2	1:B:566:ASP:OD2	2.54	0.41
1:D:496:VAL:HA	1:D:545:PHE:O	2.21	0.41
2:M:86:LYS:HA	2:M:86:LYS:HD3	1.83	0.41
2:N:497:ASP:OD2	2:N:585:TYR:OH	2.27	0.41
2:O:476:GLU:C	2:O:478:MET:H	2.28	0.41
2:O:684:ARG:HH11	2:O:685:ARG:HG2	1.85	0.41
1:A:370:ARG:HG2	1:A:370:ARG:NH1	2.31	0.41
1:A:370:ARG:HH11	1:A:370:ARG:CG	2.33	0.41
1:A:603:HIS:HA	1:A:633:ILE:O	2.21	0.41
1:B:483:THR:HB	1:B:638:PRO:HB2	2.02	0.41
1:D:28:THR:HG21	1:D:33:VAL:HG12	2.02	0.41
2:M:122:LYS:HD2	2:M:125:GLU:OE1	2.20	0.41
2:M:229:PHE:CD1	9:M:953:ACT:H2	2.56	0.41
2:M:383:PRO:HG2	2:M:469:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:391:TYR:HD2	2:O:462:ARG:HB2	1.85	0.41
2:P:281:PRO:HB3	2:P:296:GLU:OE1	2.20	0.41
2:P:383:PRO:O	2:P:469:THR:HA	2.21	0.41
2:P:488:ARG:C	2:P:490:ASP:H	2.28	0.41
2:P:496:THR:OG1	2:P:499:THR:HG23	2.20	0.41
2:O:199:LYS:HZ1	2:O:415:GLU:CD	2.23	0.41
2:O:478:MET:CE	2:O:478:MET:O	2.67	0.41
1:A:601:PRO:HD3	1:A:652:ARG:CZ	2.51	0.40
2:N:204:TYR:CE1	2:N:331:GLU:HB2	2.56	0.40
2:P:219:ALA:O	2:P:223:LEU:HG	2.21	0.40
2:P:701:ASP:N	2:P:704:ILE:HD13	2.36	0.40
1:A:436:LEU:HD12	1:A:547:MET:HE3	2.03	0.40
1:B:298:MET:HE1	1:B:402:ARG:CG	2.51	0.40
1:B:370:ARG:NE	11:B:2057:HOH:O	2.30	0.40
1:D:235:ILE:HG23	1:D:597:SER:OG	2.21	0.40
2:N:372:ASP:OD1	2:N:373:ILE:N	2.47	0.40
2:N:560:ILE:N	2:N:560:ILE:CD1	2.85	0.40
1:C:216:VAL:HG12	1:D:108:THR:HA	2.02	0.40
2:M:324:PHE:HA	2:M:413:TYR:O	2.22	0.40
2:N:10:GLY:N	11:N:1249:HOH:O	2.28	0.40
2:O:425:ILE:H	2:O:426:ASN:ND2	2.19	0.40
2:O:612:MET:HB3	2:O:669:TRP:HB3	2.03	0.40
2:P:358:GLU:O	2:P:359:SER:HB3	2.21	0.40
2:P:720:HIS:HA	2:P:721:PRO:HD2	1.93	0.40
1:A:482:LEU:HD22	1:A:482:LEU:HA	1.90	0.40
2:M:641:THR:O	2:M:642:PRO:C	2.64	0.40
2:N:721:PRO:O	2:N:725:MET:HG3	2.21	0.40
2:O:144:PHE:CE1	2:O:205:ILE:HG12	2.56	0.40
2:P:342:MET:HB3	2:P:382:LEU:O	2.22	0.40
1:C:62:GLY:HA3	3:C:700:SF4:S4	2.61	0.40
2:M:675:LYS:NZ	2:M:699:ILE:O	2.43	0.40
2:O:340:VAL:HG21	2:O:441:PHE:CZ	2.48	0.40
2:P:66:ARG:O	2:P:70:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

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	676/673 (100%)	651 (96%)	23 (3%)	2 (0%)	36	34
1	B	678/673 (101%)	653 (96%)	23 (3%)	2 (0%)	36	34
1	C	674/673 (100%)	648 (96%)	25 (4%)	1 (0%)	48	50
1	D	671/673 (100%)	645 (96%)	22 (3%)	4 (1%)	21	15
2	M	730/728 (100%)	697 (96%)	28 (4%)	5 (1%)	18	13
2	N	727/728 (100%)	700 (96%)	22 (3%)	5 (1%)	18	13
2	O	727/728 (100%)	650 (89%)	51 (7%)	26 (4%)	2	0
2	P	728/728 (100%)	684 (94%)	37 (5%)	7 (1%)	12	8
All	All	5611/5604 (100%)	5328 (95%)	231 (4%)	52 (1%)	14	9

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	B	267	ASN
1	B	415	ASN
1	D	415	ASN
1	D	416	ARG
2	N	316	ILE
2	O	315	LYS
2	O	335	LYS
2	O	395	MET
2	O	426	ASN
2	O	427	TRP
2	O	727	PRO
2	O	728	ILE
2	P	359	SER
1	A	415	ASN
1	C	267	ASN
1	D	267	ASN

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Mol	Chain	Res	Type
1	D	417	PRO
2	M	315	LYS
2	N	315	LYS
2	O	187	ASP
2	O	360	GLU
2	O	363	ASP
2	O	366	ILE
2	O	396	GLN
2	O	397	ALA
2	O	400	GLU
2	O	423	ARG
2	O	449	VAL
2	O	470	ASP
2	O	722	ALA
2	P	458	ALA
2	M	187	ASP
2	M	596	GLY
2	N	187	ASP
2	O	348	PRO
2	O	361	ILE
2	O	436	ALA
2	P	187	ASP
2	M	228	MET
2	N	228	MET
2	N	596	GLY
2	O	316	ILE
2	O	364	GLY
2	O	553	LYS
2	P	596	GLY
2	P	345	ASN
2	M	658	ILE
2	P	489	ASP
2	O	658	ILE
2	O	726	ASP
2	P	658	ILE

5.3.2 Protein sidechains ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	547/542 (101%)	529 (97%)	18 (3%)	33	34
1	B	549/542 (101%)	533 (97%)	16 (3%)	37	39
1	C	543/542 (100%)	530 (98%)	13 (2%)	43	47
1	D	541/542 (100%)	524 (97%)	17 (3%)	35	37
2	M	614/610 (101%)	576 (94%)	38 (6%)	16	12
2	N	611/610 (100%)	571 (94%)	40 (6%)	15	11
2	O	611/610 (100%)	537 (88%)	74 (12%)	5	2
2	P	612/610 (100%)	558 (91%)	54 (9%)	9	5
All	All	4628/4608 (100%)	4358 (94%)	270 (6%)	18	14

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	159	VAL
1	A	206	PHE
1	A	284	ASN
1	A	298	MET
1	A	318	THR
1	A	395	GLU
1	A	411	ARG
1	A	416	ARG
1	A	418	VAL
1	A	466	LEU
1	A	470	CYS
1	A	482	LEU
1	A	518	THR
1	A	538	GLU
1	A	647	ASP
1	A	656	LEU
1	A	661	GLU
1	B	23	LYS
1	B	27	ARG
1	B	77	ARG
1	B	206	PHE
1	B	284	ASN
1	B	411	ARG
1	B	413	GLU

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Mol	Chain	Res	Type
1	B	415	ASN
1	B	416	ARG
1	B	427	VAL
1	B	466	LEU
1	B	470	CYS
1	B	482	LEU
1	B	518	THR
1	B	539	ILE
1	B	656	LEU
1	C	23	LYS
1	C	27	ARG
1	C	81[A]	THR
1	C	81[B]	THR
1	C	206	PHE
1	C	291	ILE
1	C	359	SER
1	C	466	LEU
1	C	482	LEU
1	C	600	VAL
1	C	647	ASP
1	C	656	LEU
1	C	664	GLU
1	D	53	VAL
1	D	82	ASP
1	D	155	GLU
1	D	196	GLU
1	D	206	PHE
1	D	284	ASN
1	D	299	GLU
1	D	339	LEU
1	D	395	GLU
1	D	415	ASN
1	D	427	VAL
1	D	438	LYS
1	D	518	THR
1	D	530	ARG
1	D	539	ILE
1	D	656	LEU
1	D	664	GLU
2	M	14	GLU
2	M	66	ARG
2	M	127	LEU

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Mol	Chain	Res	Type
2	M	152	THR
2	M	169	LEU
2	M	171	LYS
2	M	205	ILE
2	M	238[A]	GLU
2	M	238[B]	GLU
2	M	245	ARG
2	M	247	ARG
2	M	249	ARG
2	M	262	LYS
2	M	315	LYS
2	M	318	LEU
2	M	340	VAL
2	M	354	ARG
2	M	373	ILE
2	M	378	GLU
2	M	381	LYS
2	M	382	LEU
2	M	393	ARG
2	M	422	GLN
2	M	424	ASN
2	M	426	ASN
2	M	448	LEU
2	M	471	GLU
2	M	486	LYS
2	M	492	MET
2	M	571	LEU
2	M	604	ILE
2	M	672	LYS
2	M	674	LEU
2	M	681	GLU
2	M	702	GLU
2	M	704	ILE
2	M	723	LEU
2	M	726	ASP
2	N	6	LYS
2	N	66	ARG
2	N	89	GLN
2	N	124	ASP
2	N	152	THR
2	N	174	LYS
2	N	185	ILE

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Mol	Chain	Res	Type
2	N	198	VAL
2	N	247	ARG
2	N	249	ARG
2	N	262	LYS
2	N	284	GLU
2	N	312	LYS
2	N	316	ILE
2	N	318	LEU
2	N	319	ASP
2	N	331	GLU
2	N	332	SER
2	N	335	LYS
2	N	354	ARG
2	N	373	ILE
2	N	381	LYS
2	N	424	ASN
2	N	425	ILE
2	N	426	ASN
2	N	448	LEU
2	N	475	LYS
2	N	492	MET
2	N	493	ARG
2	N	495	LEU
2	N	560	ILE
2	N	571	LEU
2	N	604	ILE
2	N	631	LEU
2	N	640	GLN
2	N	672	LYS
2	N	674	LEU
2	N	702	GLU
2	N	704	ILE
2	N	729	MET
2	O	2	THR
2	O	3	ASP
2	O	6	LYS
2	O	14	GLU
2	O	64	VAL
2	O	66	ARG
2	O	71	GLU
2	O	125	GLU
2	O	127	LEU

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Mol	Chain	Res	Type
2	O	152	THR
2	O	166	SER
2	O	169	LEU
2	O	174	LYS
2	O	198	VAL
2	O	205	ILE
2	O	214	GLN
2	O	245	ARG
2	O	284	GLU
2	O	316	ILE
2	O	317	LYS
2	O	342	MET
2	O	345	ASN
2	O	347	THR
2	O	350	PHE
2	O	351	GLU
2	O	352	LEU
2	O	356	VAL
2	O	360	GLU
2	O	362	THR
2	O	366	ILE
2	O	367	GLU
2	O	376	ILE
2	O	378	GLU
2	O	380	SER
2	O	393	ARG
2	O	399	PHE
2	O	406	ARG
2	O	422	GLN
2	O	423	ARG
2	O	424	ASN
2	O	425	ILE
2	O	426	ASN
2	O	440	ARG
2	O	442	LYS
2	O	455	GLU
2	O	460	VAL
2	O	473	LYS
2	O	478	MET
2	O	484	LYS
2	O	495	LEU
2	O	497	ASP

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Mol	Chain	Res	Type
2	O	524	ARG
2	O	525	VAL
2	O	541	GLU
2	O	575	SER
2	O	579	LEU
2	O	581	GLN
2	O	586	THR
2	O	609	ASN
2	O	622	THR
2	O	631	LEU
2	O	647	ILE
2	O	672	LYS
2	O	685	ARG
2	O	687	VAL
2	O	689	GLU
2	O	693	GLU
2	O	704	ILE
2	O	718	LYS
2	O	723	LEU
2	O	724	THR
2	O	725	MET
2	O	728	ILE
2	O	729	MET
2	P	9	GLU
2	P	66	ARG
2	P	124	ASP
2	P	125	GLU
2	P	152	THR
2	P	174	LYS
2	P	205	ILE
2	P	245	ARG
2	P	272	THR
2	P	284	GLU
2	P	315	LYS
2	P	317	LYS
2	P	329	GLU
2	P	331	GLU
2	P	335	LYS
2	P	342	MET
2	P	346	ARG
2	P	347	THR
2	P	362	THR

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Mol	Chain	Res	Type
2	P	365	LYS
2	P	373	ILE
2	P	405	ARG
2	P	419	HIS
2	P	422	GLN
2	P	424	ASN
2	P	428	LEU
2	P	448	LEU
2	P	462	ARG
2	P	463	VAL
2	P	466	THR
2	P	467	ILE
2	P	471	GLU
2	P	478	MET
2	P	480	VAL
2	P	483	GLU
2	P	486	LYS
2	P	493	ARG
2	P	495	LEU
2	P	502	THR
2	P	537	LYS
2	P	541	GLU
2	P	542	ILE
2	P	549	GLN
2	P	554	GLU
2	P	563	ILE
2	P	565	LYS
2	P	605	LEU
2	P	631	LEU
2	P	650	THR
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 (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	HIS
1	A	201	HIS
1	A	209	HIS

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Mol	Chain	Res	Type
1	A	217	ASN
1	A	220	HIS
1	A	275	GLN
1	A	284	ASN
1	A	454	GLN
1	A	477	GLN
1	A	515	ASN
1	B	122	HIS
1	B	201	HIS
1	B	209	HIS
1	B	217	ASN
1	B	220	HIS
1	B	260	GLN
1	B	284	ASN
1	B	447	ASN
1	B	454	GLN
1	B	477	GLN
1	B	479	ASN
1	B	639	GLN
1	C	122	HIS
1	C	201	HIS
1	C	209	HIS
1	C	220	HIS
1	C	260	GLN
1	C	275	GLN
1	C	284	ASN
1	C	443	GLN
1	C	477	GLN
1	C	479	ASN
1	D	201	HIS
1	D	209	HIS
1	D	220	HIS
1	D	260	GLN
1	D	284	ASN
1	D	293	GLN
1	D	477	GLN
1	D	503	GLN
1	D	515	ASN
2	M	211	ASN
2	M	408	HIS
2	M	422	GLN
2	M	424	ASN

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Mol	Chain	Res	Type
2	M	426	ASN
2	M	544	HIS
2	M	549	GLN
2	M	581	GLN
2	M	590	ASN
2	N	211	ASN
2	N	345	ASN
2	N	408	HIS
2	N	424	ASN
2	N	426	ASN
2	N	510	GLN
2	N	549	GLN
2	N	581	GLN
2	N	590	ASN
2	N	679	HIS
2	O	27	HIS
2	O	396	GLN
2	O	424	ASN
2	O	464	GLN
2	O	516	HIS
2	O	578	ASN
2	O	590	ASN
2	O	618	HIS
2	O	640	GLN
2	O	720	HIS
2	P	27	HIS
2	P	211	ASN
2	P	287	GLN
2	P	408	HIS
2	P	422	GLN
2	P	424	ASN
2	P	426	ASN
2	P	464	GLN
2	P	590	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	XCC	A	800	5,11,1	0,12,12	-	-	-		
9	ACT	M	953	-	1,2,3	1.24	0	0,1,3	-	-
3	SF4	P	900	2	0,12,12	-	-	-		
6	GOL	A	963	-	5,5,5	0.68	0	5,5,5	1.88	3 (60%)
5	CYN	B	900	4	1,1,1	0.58	0	-		
3	SF4	O	900	2	0,12,12	-	-	-		
4	XCC	C	800	5,11,1	0,12,12	-	-	-		
3	SF4	B	750	1	0,12,12	-	-	-		
3	SF4	N	900	2	0,12,12	-	-	-		
6	GOL	B	963	-	5,5,5	0.81	0	5,5,5	1.79	1 (20%)
3	SF4	C	750	1	0,12,12	-	-	-		
9	ACT	N	953	-	1,2,3	1.30	0	0,1,3	-	-
9	ACT	O	953	-	1,2,3	1.33	0	0,1,3	-	-
5	CYN	C	900	4	1,1,1	0.08	0	-		
3	SF4	C	700	1	0,12,12	-	-	-		
5	CYN	A	900	4	1,1,1	0.28	0	-		
9	ACT	P	953	-	1,2,3	1.37	0	0,1,3	-	-
6	GOL	C	963	-	5,5,5	0.54	0	5,5,5	1.00	0
3	SF4	A	700	1	0,12,12	-	-	-		
3	SF4	A	750	1	0,12,12	-	-	-		
4	XCC	B	800	5,11,1	0,12,12	-	-	-		
4	XCC	D	800	11,1	0,12,12	-	-	-		
3	SF4	M	900	2	0,12,12	-	-	-		
5	CYN	D	900	-	1,1,1	0.16	0	-		
6	GOL	D	963	-	5,5,5	0.69	0	5,5,5	1.43	1 (20%)
3	SF4	D	750	1	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	C	750	1	-	-	0/6/5/5
3	SF4	A	700	1	-	-	0/6/5/5
3	SF4	O	900	2	-	-	0/6/5/5
4	XCC	D	800	11,1	-	-	0/4/4/4
4	XCC	A	800	5,11,1	-	-	0/4/4/4
3	SF4	M	900	2	-	-	0/6/5/5
3	SF4	C	700	1	-	-	0/6/5/5
4	XCC	C	800	5,11,1	-	-	0/4/4/4
3	SF4	B	750	1	-	-	0/6/5/5
3	SF4	A	750	1	-	-	0/6/5/5
3	SF4	P	900	2	-	-	0/6/5/5
3	SF4	N	900	2	-	-	0/6/5/5
6	GOL	C	963	-	-	3/4/4/4	-
6	GOL	A	963	-	-	2/4/4/4	-
6	GOL	B	963	-	-	1/4/4/4	-
3	SF4	D	750	1	-	-	0/6/5/5
4	XCC	B	800	5,11,1	-	-	0/4/4/4
6	GOL	D	963	-	-	4/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	963	GOL	O2-C2-C3	-2.58	98.50	109.18
6	D	963	GOL	O1-C1-C2	-2.50	99.10	110.38
6	A	963	GOL	O1-C1-C2	-2.47	99.24	110.38
6	A	963	GOL	O2-C2-C3	-2.28	99.73	109.18
6	A	963	GOL	O3-C3-C2	-2.17	100.62	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

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

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	953	ACT	1	0
6	A	963	GOL	1	0
9	N	953	ACT	3	0
9	O	953	ACT	1	0
5	C	900	CYN	3	0
3	C	700	SF4	1	0
5	A	900	CYN	2	0
9	P	953	ACT	1	0
6	C	963	GOL	4	0
5	D	900	CYN	1	0
6	D	963	GOL	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	673/673 (100%)	-0.34	6 (0%)	81 83	8, 24, 42, 62	5 (0%)
1	B	673/673 (100%)	-0.50	7 (1%)	79 82	7, 22, 39, 66	7 (1%)
1	C	673/673 (100%)	-0.30	1 (0%)	92 93	15, 26, 41, 57	3 (0%)
1	D	673/673 (100%)	-0.17	8 (1%)	76 79	19, 28, 43, 62	0
2	M	728/728 (100%)	0.09	23 (3%)	50 54	13, 31, 58, 76	4 (0%)
2	N	728/728 (100%)	0.02	33 (4%)	38 43	11, 30, 57, 71	1 (0%)
2	O	728/728 (100%)	1.65	277 (38%)	1 1	17, 62, 88, 123	1 (0%)
2	P	728/728 (100%)	0.81	140 (19%)	3 4	13, 45, 79, 107	2 (0%)
All	All	5604/5604 (100%)	0.18	495 (8%)	15 17	7, 29, 74, 123	23 (0%)

All (495) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	728	ILE	7.6
2	O	450	ALA	7.2
2	O	366	ILE	6.2
2	O	481	ALA	6.0
2	O	427	TRP	6.0
2	O	340	VAL	5.9
2	O	356	VAL	5.6
2	P	492	MET	5.5
2	O	449	VAL	5.4
2	O	534	LEU	5.3
2	O	480	VAL	5.2
2	P	494	GLY	5.2
2	O	715	LEU	5.1
2	O	428	LEU	5.1
2	O	712	LEU	5.1
2	O	463	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	O	683	VAL	5.0
2	O	361	ILE	5.0
2	O	563	ILE	4.9
2	O	402	VAL	4.9
2	O	465	VAL	4.9
2	O	725	MET	4.8
2	O	447	ILE	4.8
2	O	567	VAL	4.8
2	P	427	TRP	4.7
2	O	339	TYR	4.7
2	O	460	VAL	4.7
2	O	380	SER	4.7
2	P	356	VAL	4.7
2	O	397	ALA	4.7
2	M	729	MET	4.7
2	O	474	VAL	4.7
2	O	353	VAL	4.6
2	M	640[A]	GLN	4.6
2	P	485	TYR	4.5
2	O	387	LEU	4.5
2	O	350	PHE	4.4
2	O	399	PHE	4.4
2	P	728	ILE	4.4
2	O	469	THR	4.4
2	O	495	LEU	4.4
2	O	369	ILE	4.4
2	O	723	LEU	4.4
2	P	340	VAL	4.3
2	O	691	LEU	4.3
2	O	362	THR	4.3
2	O	316	ILE	4.3
2	O	459	ILE	4.3
2	O	407	ILE	4.2
2	O	488	ARG	4.2
2	O	458	ALA	4.2
2	P	387	LEU	4.2
2	O	564	TRP	4.2
2	O	559	PRO	4.2
2	O	472	ALA	4.2
2	P	481	ALA	4.2
2	O	525	VAL	4.2
2	O	418	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
2	O	467	ILE	4.1
2	O	542	ILE	4.1
1	D	417	PRO	4.1
2	O	424	ASN	4.1
2	O	382	LEU	4.1
2	M	316	ILE	4.1
2	O	425	ILE	4.1
2	O	485	TYR	4.1
2	O	574	ALA	4.0
2	O	700	ALA	4.0
2	P	729	MET	4.0
2	O	687	VAL	4.0
2	P	353	VAL	4.0
2	O	708	VAL	4.0
2	P	339	TYR	4.0
2	O	333	ILE	4.0
2	O	390	ILE	4.0
2	O	658	ILE	4.0
2	P	316	ILE	4.0
2	O	381	LYS	4.0
2	O	456	PHE	3.9
2	O	647	ILE	3.9
2	O	368	VAL	3.9
2	O	388	VAL	3.9
2	O	468	PHE	3.9
2	O	491	ARG	3.9
2	O	426	ASN	3.9
2	O	355	THR	3.9
2	P	496	THR	3.9
2	O	477	TYR	3.8
2	O	384	LEU	3.8
2	P	480	VAL	3.8
2	O	379	GLY	3.8
2	O	486	LYS	3.8
2	O	322	ILE	3.7
2	O	713	PRO	3.7
2	N	316	ILE	3.7
2	P	333	ILE	3.7
2	O	417	LEU	3.7
2	O	531	VAL	3.7
2	O	560	ILE	3.7
2	O	639	THR	3.7

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Mol	Chain	Res	Type	RSRZ
2	P	477	TYR	3.7
2	M	318	LEU	3.7
2	O	343	GLY	3.7
2	P	382	LEU	3.6
2	P	371	PRO	3.6
2	P	484	LYS	3.6
2	O	410	PHE	3.6
2	O	711	ILE	3.6
2	O	714	TYR	3.6
1	B	539	ILE	3.6
2	O	476	GLU	3.6
2	O	395	MET	3.6
2	O	557	ILE	3.6
2	P	425	ILE	3.6
2	O	348	PRO	3.6
2	O	352	LEU	3.6
2	P	495	LEU	3.6
2	O	685	ARG	3.6
2	P	486	LYS	3.6
2	O	389	ASP	3.5
2	O	492	MET	3.5
2	O	729	MET	3.5
2	O	500	VAL	3.5
1	A	415	ASN	3.5
2	P	350	PHE	3.5
2	P	352	LEU	3.5
2	N	729	MET	3.5
2	O	344	GLY	3.5
2	P	421	GLY	3.5
2	O	540	TYR	3.5
2	P	391	TYR	3.5
2	N	315	LYS	3.4
2	O	484	LYS	3.4
2	O	478	MET	3.4
2	O	377	PRO	3.4
2	O	499	THR	3.4
2	O	724	THR	3.4
1	D	416	ARG	3.4
2	O	519	ILE	3.4
2	O	318	LEU	3.4
2	O	587	LEU	3.4
2	O	371	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	O	401	GLY	3.3
2	P	459	ILE	3.3
2	O	533	TRP	3.3
2	O	504	TYR	3.3
2	P	474	VAL	3.3
2	O	473	LYS	3.3
2	O	585	TYR	3.3
2	P	349	ALA	3.3
2	O	670	MET	3.3
2	N	474	VAL	3.2
2	O	579	LEU	3.2
2	P	314	THR	3.2
2	O	623	PRO	3.2
2	O	342	MET	3.2
2	O	475	LYS	3.2
2	P	335	LYS	3.2
2	O	699	ILE	3.2
2	P	369	ILE	3.2
2	P	390	ILE	3.2
2	P	488	ARG	3.2
2	P	402	VAL	3.2
2	O	722	ALA	3.2
2	O	335	LYS	3.2
2	N	313	LEU	3.1
2	O	373	ILE	3.1
2	O	490	ASP	3.1
2	O	570	TYR	3.1
2	O	547	PRO	3.1
2	O	727	PRO	3.1
2	O	434	ALA	3.1
2	O	653	VAL	3.1
2	P	660	ALA	3.1
2	P	313	LEU	3.1
2	P	373	ILE	3.1
2	O	496	THR	3.1
2	O	457	PRO	3.1
2	M	472	ALA	3.1
1	B	537	ILE	3.1
2	O	386	ILE	3.1
2	O	347	THR	3.1
2	O	595	CYS	3.1
2	O	432	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	P	460	VAL	3.1
1	D	539	ILE	3.1
2	N	373	ILE	3.1
2	O	376	ILE	3.1
2	O	464	GLN	3.1
2	P	552	PRO	3.0
2	O	545	ALA	3.0
2	M	474	VAL	3.0
2	P	343	GLY	3.0
2	P	491	ARG	3.0
2	P	478	MET	3.0
2	O	435	VAL	3.0
2	P	336	GLY	3.0
2	O	487	GLU	3.0
2	M	314	THR	3.0
2	O	586	THR	3.0
2	O	641	THR	3.0
2	P	348	PRO	3.0
2	P	457	PRO	3.0
2	O	651	TYR	3.0
2	P	403	LEU	3.0
2	P	567	VAL	3.0
2	O	613	ILE	3.0
2	O	544	HIS	3.0
2	O	439	PHE	3.0
2	P	418	TRP	3.0
2	O	448	LEU	2.9
2	O	605	LEU	2.9
2	O	394	LYS	2.9
2	O	314	THR	2.9
2	O	461	ASP	2.9
2	P	362	THR	2.9
2	O	657	PHE	2.9
2	O	594	SER	2.9
2	O	665	ALA	2.9
2	N	466	THR	2.9
2	P	377	PRO	2.9
2	O	482	ARG	2.9
2	O	349	ALA	2.9
2	M	728	ILE	2.9
2	O	551	ILE	2.9
2	P	361	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	N	317	LYS	2.9
2	O	695	PHE	2.9
2	O	719	GLY	2.9
1	A	416	ARG	2.8
2	O	602	MET	2.8
2	P	342	MET	2.8
2	P	557	ILE	2.8
2	O	721	PRO	2.8
2	P	354	ARG	2.8
2	O	638	GLY	2.8
2	N	318	LEU	2.8
2	O	508	LEU	2.8
2	N	367	GLU	2.8
2	O	149	VAL	2.8
2	O	520	VAL	2.8
2	O	383	PRO	2.8
2	O	704	ILE	2.8
2	P	315	LYS	2.8
2	P	456	PHE	2.8
2	O	530	ALA	2.8
2	P	574	ALA	2.8
2	M	382	LEU	2.8
2	O	441	PHE	2.8
2	O	444	TYR	2.8
2	M	313	LEU	2.8
2	O	655	LYS	2.8
2	O	635	ILE	2.8
2	O	696	ILE	2.8
1	D	368	HIS	2.7
2	O	364	GLY	2.7
2	O	526	GLY	2.7
2	P	385	GLY	2.7
2	O	503	PHE	2.7
2	O	391	TYR	2.7
2	O	552	PRO	2.7
2	O	671	PRO	2.7
2	O	517	VAL	2.7
2	P	376	ILE	2.7
2	P	467	ILE	2.7
2	P	563	ILE	2.7
2	O	367	GLU	2.7
2	O	566	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	N	638	GLY	2.7
2	P	401	GLY	2.7
2	N	2	THR	2.7
2	O	320	LEU	2.7
2	O	650	THR	2.7
2	P	534	LEU	2.7
2	P	579	LEU	2.7
2	P	623	PRO	2.7
2	N	480	VAL	2.7
2	O	338	MET	2.7
2	O	645	MET	2.7
2	O	668	VAL	2.7
2	P	483	GLU	2.7
2	O	494	GLY	2.7
2	O	646	GLY	2.7
2	P	712	LEU	2.7
2	O	522	PRO	2.7
1	B	20	MET	2.7
2	P	430	VAL	2.7
2	O	583	CYS	2.7
2	O	317	LYS	2.7
2	O	718	LYS	2.7
2	P	640	GLN	2.6
1	A	661	GLU	2.6
2	P	458	ALA	2.6
2	O	707	THR	2.6
2	P	503	PHE	2.6
2	O	422	GLN	2.6
2	P	533	TRP	2.6
2	O	497	ASP	2.6
2	P	487	GLU	2.6
2	P	420	THR	2.6
2	N	348	PRO	2.6
2	O	313	LEU	2.6
2	P	584	LEU	2.6
2	P	723	LEU	2.6
2	O	429	ARG	2.6
2	O	493	ARG	2.6
2	N	360	GLU	2.6
2	P	476	GLU	2.6
2	O	648	GLY	2.6
1	D	415	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
2	O	593	THR	2.6
2	N	468	PHE	2.5
2	N	370	GLY	2.5
2	O	336	GLY	2.5
2	O	662	GLY	2.5
2	P	466	THR	2.5
2	P	713	PRO	2.5
2	P	727	PRO	2.5
2	O	571	LEU	2.5
2	O	678	LEU	2.5
2	O	471	GLU	2.5
2	P	338	MET	2.5
2	O	582	VAL	2.5
2	P	551	ILE	2.5
1	B	416	ARG	2.5
2	P	482	ARG	2.5
2	O	398	ASP	2.5
2	O	470	ASP	2.5
2	P	124	ASP	2.5
2	O	400	GLU	2.5
2	O	606	PRO	2.5
2	P	431	SER	2.5
2	O	698	LYS	2.5
2	O	664	ILE	2.5
2	P	465	VAL	2.5
2	O	659	SER	2.5
1	A	368	HIS	2.5
2	O	516	HIS	2.5
2	M	376	ILE	2.5
2	O	357	SER	2.4
2	P	347	THR	2.4
1	B	535	ALA	2.4
2	O	584	LEU	2.4
2	O	674	LEU	2.4
2	P	475	LYS	2.4
1	B	536	ASN	2.4
2	M	693	GLU	2.4
2	N	376	ILE	2.4
2	O	604	ILE	2.4
2	P	341	GLU	2.4
2	P	366	ILE	2.4
2	N	371	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	P	383	PRO	2.4
2	O	393	ARG	2.4
2	O	553	LYS	2.4
2	O	483	GLU	2.4
2	O	667	ILE	2.4
2	P	388	VAL	2.4
2	M	639	THR	2.4
2	N	314	THR	2.4
2	O	442	LYS	2.4
2	O	451	LYS	2.4
2	O	596	GLY	2.4
2	P	461	ASP	2.4
2	O	592	MET	2.4
2	P	683	VAL	2.4
2	N	426	ASN	2.3
2	N	495	LEU	2.3
2	O	527	LEU	2.3
2	P	555	GLY	2.3
2	M	124	ASP	2.3
2	O	452	MET	2.3
2	O	611	ILE	2.3
2	O	420	THR	2.3
2	O	466	THR	2.3
2	P	573	THR	2.3
2	O	351	GLU	2.3
2	N	470	ASP	2.3
2	O	726	ASP	2.3
2	P	389	ASP	2.3
2	O	423	ARG	2.3
2	M	335	LYS	2.3
2	P	682	PHE	2.3
2	O	716	GLU	2.3
2	O	502	THR	2.3
2	P	469	THR	2.3
2	P	472	ALA	2.3
2	O	354	ARG	2.3
2	O	438	GLY	2.3
2	O	489	ASP	2.3
2	O	572	TYR	2.3
2	P	334	ARG	2.3
2	P	429	ARG	2.3
2	O	453	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	O	479	GLU	2.3
2	P	399	PHE	2.3
2	O	601	ILE	2.3
2	O	507	VAL	2.3
2	O	568	ASN	2.3
2	O	694	ASP	2.3
2	O	637	GLY	2.3
2	P	379	GLY	2.3
2	P	432	LYS	2.3
2	O	403	LEU	2.3
2	O	151	TRP	2.3
2	P	468	PHE	2.2
2	P	386	ILE	2.2
2	P	560	ILE	2.2
2	O	315	LYS	2.2
1	C	20	MET	2.2
2	N	387	LEU	2.2
2	P	428	LEU	2.2
2	M	681	GLU	2.2
2	P	564	TRP	2.2
2	O	229	PHE	2.2
2	O	524	ARG	2.2
2	O	682	PHE	2.2
2	O	321	PRO	2.2
2	P	639	THR	2.2
1	B	540	GLY	2.2
1	D	304	ALA	2.2
2	P	384	LEU	2.2
2	N	377	PRO	2.2
2	N	469	THR	2.2
1	D	82	ASP	2.2
2	O	363	ASP	2.2
2	O	433	ASP	2.2
2	P	711	ILE	2.2
2	M	719	GLY	2.2
2	O	392	GLY	2.2
2	O	562	GLY	2.2
2	N	472	ALA	2.2
2	O	679	HIS	2.2
2	O	518	CYS	2.2
2	P	583	CYS	2.2
2	O	686	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	572	TYR	2.2
2	O	6	LYS	2.2
2	P	345	ASN	2.2
2	O	669	TRP	2.2
2	O	706	THR	2.2
2	P	499	THR	2.2
2	P	541	GLU	2.1
1	D	446	GLN	2.1
2	P	364	GLY	2.1
2	P	684[A]	ARG	2.1
2	O	16	LYS	2.1
2	P	424	ASN	2.1
2	P	360	GLU	2.1
2	M	469	THR	2.1
2	O	642	PRO	2.1
2	M	696	ILE	2.1
2	O	430	VAL	2.1
2	O	663	GLY	2.1
2	M	715	LEU	2.1
2	O	359	SER	2.1
2	P	400	GLU	2.1
2	M	726	ASP	2.1
2	P	490	ASP	2.1
2	O	573	THR	2.1
2	N	15	GLY	2.1
2	O	652	ILE	2.1
2	P	462	ARG	2.1
2	P	704	ILE	2.1
2	O	644	PHE	2.1
2	P	582	VAL	2.1
2	O	536	ALA	2.1
2	O	505	SER	2.1
2	P	571	LEU	2.1
2	O	612	MET	2.1
2	O	13	PRO	2.1
2	O	684	ARG	2.1
2	N	379	GLY	2.1
2	O	705	GLY	2.1
2	P	15	GLY	2.1
2	P	381	LYS	2.1
2	P	407	ILE	2.1
2	P	542	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	463	VAL	2.1
2	O	538	ALA	2.1
2	P	397	ALA	2.1
2	P	700	ALA	2.1
2	N	639	THR	2.0
2	P	559	PRO	2.0
2	P	562	GLY	2.0
1	A	539	ILE	2.0
2	M	333	ILE	2.0
2	N	361	ILE	2.0
2	N	425	ILE	2.0
2	O	332	SER	2.0
2	M	691	LEU	2.0
2	N	3	ASP	2.0
2	P	355	THR	2.0
1	A	526	GLY	2.0
2	O	555	GLY	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($\text{\AA}^2$)	Q<0.9
9	ACT	P	953	3/4	0.86	0.41	75,75,76,76	0
10	NA	P	730	1/1	0.86	0.10	35,35,35,35	0
6	GOL	A	963	6/6	0.88	0.12	26,30,37,38	0
6	GOL	B	963	6/6	0.88	0.15	27,37,38,44	0
9	ACT	N	953	3/4	0.89	0.33	71,71,71,71	0
10	NA	O	730	1/1	0.89	0.08	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	ACT	O	953	3/4	0.89	0.34	109,109,109,109	0
6	GOL	D	963	6/6	0.90	0.12	38,43,45,45	0
6	GOL	C	963	6/6	0.90	0.14	50,53,54,55	0
9	ACT	M	953	3/4	0.91	0.29	55,55,56,56	0
5	CYN	C	900	2/2	0.91	0.32	31,31,31,33	0
3	SF4	O	900	8/8	0.94	0.07	57,60,62,64	0
5	CYN	D	900	2/2	0.94	0.24	42,42,42,43	0
5	CYN	A	900	2/2	0.94	0.23	31,31,31,32	0
5	CYN	B	900	2/2	0.96	0.15	25,25,25,25	0
10	NA	N	730	1/1	0.96	0.04	26,26,26,26	0
10	NA	M	1	1/1	0.97	0.04	28,28,28,28	0
8	NI	O	951	1/1	0.97	0.08	66,66,66,66	0
4	XCC	D	800	9/9	0.98	0.04	27,30,36,36	0
7	CU1	O	950	1/1	0.98	0.07	73,73,73,73	0
7	CU1	P	950	1/1	0.98	0.06	49,49,49,49	0
3	SF4	P	900	8/8	0.99	0.04	38,41,42,42	0
7	CU1	M	950	1/1	0.99	0.03	35,35,35,35	0
7	CU1	N	950	1/1	0.99	0.03	34,34,34,34	0
4	XCC	A	800	9/9	0.99	0.03	21,22,25,26	0
4	XCC	B	800	9/9	0.99	0.03	18,19,24,26	0
4	XCC	C	800	9/9	0.99	0.03	19,25,28,31	0
8	NI	P	951	1/1	0.99	0.05	41,41,41,41	0
3	SF4	A	750	8/8	0.99	0.03	17,17,18,19	0
3	SF4	B	750	8/8	0.99	0.02	16,16,18,18	0
3	SF4	C	700	8/8	0.99	0.04	24,29,31,31	0
3	SF4	C	750	8/8	0.99	0.03	26,27,28,29	0
3	SF4	D	750	8/8	0.99	0.04	24,24,26,26	0
3	SF4	M	900	8/8	0.99	0.03	20,22,23,23	0
3	SF4	N	900	8/8	0.99	0.02	20,23,24,25	0
3	SF4	A	700	8/8	0.99	0.03	16,17,19,20	0
8	NI	M	951	1/1	1.00	0.01	24,24,24,24	0
8	NI	N	951	1/1	1.00	0.01	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.