



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:46 PM UTC

PDB ID : 1OAD / pdb_00001oad
Title : Glucose isomerase from Streptomyces rubiginosus in P21212 crystal form
Authors : Ramagopal, U.A.; Dauter, M.; Dauter, Z.
Deposited on : 2003-01-08
Resolution : 1.50 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

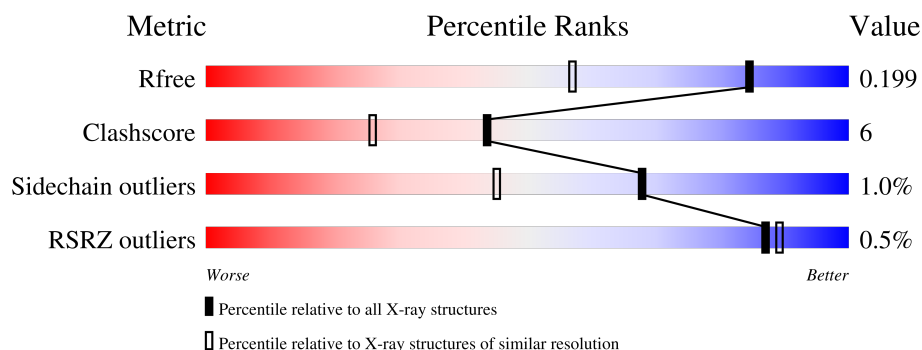
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	388	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>44%</div> <div>.</div> </div> </div>
1	B	388	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>.</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7120 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 XYLOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	5	0
			3060	1922	552	577	9			
1	B	386	Total	C	N	O	S	0	13	0
			3095	1941	560	585	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLU	GLN	conflict	UNP P24300
B	21	GLU	GLN	conflict	UNP P24300

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

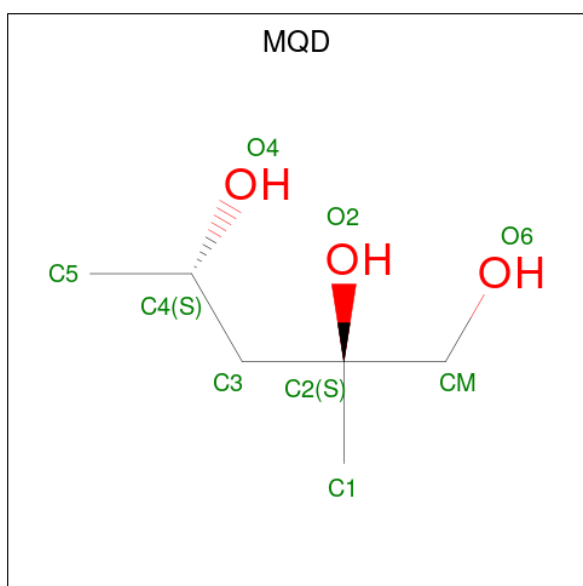
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 2-METHYLPENTANE-1,2,4-TRIOL (CCD ID: MQD) (formula: $C_6H_{14}O_3$).



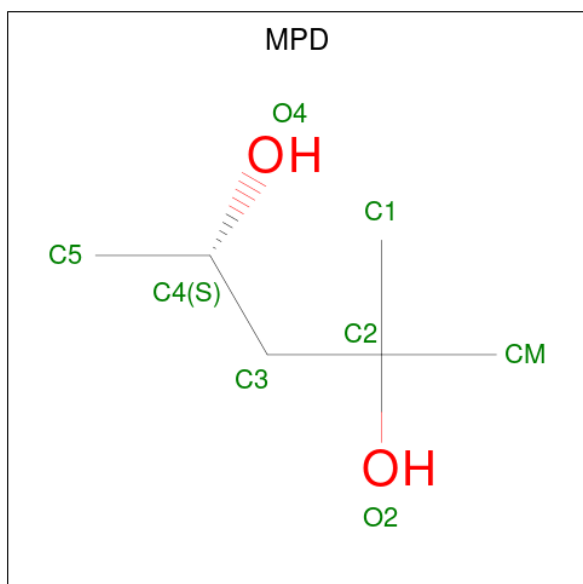
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	6	3		
5	B	1	Total	C	O	0	0
			9	6	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	474	Total 474	O 474	1	0
8	B	437	Total 437	O 437	0	0

A344	D345	G346	L347	Q348	A349	L350
R354	S355	A356	V362	D363	A364	A365
R368	A371	R374	L375	D376	Q377	L378
D381	H382	R387	GLY			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.45Å 129.59Å 78.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.50 20.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-1.50) 97.9 (20.00-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.71 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.163 , 0.186 (Not available) , 0.199	Depositor DCC
R_{free} test set	7880 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7120	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MQD, MN, TRS, MRD, MG, MPD

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	1.79	42/3158 (1.3%)	2.52	224/4270 (5.2%)
1	B	1.70	31/3231 (1.0%)	2.48	259/4368 (5.9%)
All	All	1.74	73/6389 (1.1%)	2.50	483/8638 (5.6%)

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ARG	NE-CZ	9.42	1.43	1.33
1	A	201	ALA	C-O	7.65	1.33	1.24
1	A	14	GLY	C-O	7.34	1.31	1.23
1	A	307	MET	C-N	7.20	1.43	1.33
1	B	220	HIS	CE1-NE2	7.05	1.39	1.32
1	B	196	VAL	C-O	7.01	1.32	1.24
1	B	102	GLY	C-N	6.90	1.39	1.33
1	A	189	GLY	C-N	6.83	1.42	1.33
1	A	253[A]	LYS	C-O	6.55	1.30	1.24
1	A	253[B]	LYS	C-O	6.55	1.30	1.24
1	B	24	ASP	CA-C	6.53	1.58	1.52
1	B	17	THR	C-O	6.47	1.29	1.23
1	B	378	LEU	C-N	6.44	1.42	1.33
1	B	157	ARG	CZ-NH2	6.38	1.41	1.33
1	A	213	GLY	CA-C	6.37	1.60	1.51
1	B	267	ALA	C-O	6.32	1.32	1.24
1	B	371	ALA	C-N	6.30	1.43	1.33
1	A	239	GLY	C-N	6.17	1.42	1.33
1	A	286	PHE	C-N	6.13	1.41	1.33
1	B	212	TYR	N-CA	6.09	1.53	1.46
1	A	312	ILE	C-N	6.07	1.42	1.34
1	B	248	GLY	CA-C	6.07	1.57	1.52
1	B	259	ARG	C-N	6.00	1.41	1.33
1	A	102	GLY	N-CA	5.96	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	GLY	C-O	5.95	1.30	1.24
1	A	290	PRO	CA-C	5.94	1.57	1.52
1	A	113	ARG	NE-CZ	5.93	1.39	1.33
1	A	220	HIS	CE1-NE2	5.89	1.38	1.32
1	B	303	ALA	N-CA	5.88	1.53	1.46
1	A	244	ILE	CA-CB	-5.84	1.46	1.55
1	A	198	HIS	ND1-CE1	5.83	1.38	1.32
1	B	253[A]	LYS	C-O	5.77	1.29	1.24
1	B	253[B]	LYS	C-O	5.77	1.29	1.24
1	B	321	ARG	CZ-NH2	5.74	1.41	1.33
1	A	298	GLY	CA-C	5.74	1.59	1.51
1	A	103	GLY	CA-C	5.73	1.59	1.51
1	A	305	GLY	CA-C	5.73	1.58	1.52
1	B	220	HIS	CG-CD2	5.72	1.42	1.35
1	A	311	LEU	C-N	5.71	1.41	1.33
1	A	234	GLN	C-O	5.68	1.30	1.24
1	A	201	ALA	CA-C	-5.66	1.45	1.52
1	A	197	GLY	C-O	5.66	1.30	1.23
1	A	95	THR	C-O	5.62	1.30	1.24
1	A	288	PHE	N-CA	5.62	1.53	1.45
1	A	276	GLU	C-O	5.62	1.30	1.24
1	B	247	ASN	C-N	5.61	1.40	1.33
1	A	215	ASN	CA-C	5.59	1.58	1.52
1	B	102	GLY	N-CA	5.59	1.50	1.45
1	B	153	ASP	C-N	5.57	1.41	1.33
1	B	265	LEU	C-O	5.57	1.30	1.24
1	B	374	ARG	C-N	5.49	1.40	1.33
1	B	291	PRO	C-N	5.45	1.41	1.33
1	A	259	ARG	NE-CZ	5.43	1.39	1.33
1	A	248	GLY	N-CA	5.39	1.50	1.44
1	A	252	ILE	CA-C	-5.39	1.47	1.52
1	B	356	ALA	C-O	5.38	1.31	1.24
1	B	274	LEU	C-O	5.37	1.30	1.24
1	A	248	GLY	CA-C	5.29	1.56	1.52
1	B	14	GLY	C-O	5.29	1.29	1.23
1	B	136	ALA	N-CA	5.26	1.52	1.46
1	B	234	GLN	C-O	5.24	1.30	1.24
1	A	102	GLY	C-O	-5.24	1.18	1.23
1	A	109	ARG	CZ-NH2	5.24	1.40	1.33
1	A	220	HIS	CG-CD2	5.24	1.41	1.35
1	B	331	ARG	C-N	5.21	1.41	1.34
1	B	260	PHE	CA-C	5.21	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	ASP	N-CA	-5.15	1.40	1.46
1	A	217	GLU	CD-OE2	5.11	1.35	1.25
1	A	300	TRP	C-N	5.09	1.40	1.33
1	A	297	ASP	C-N	5.07	1.40	1.33
1	A	220	HIS	C-O	5.00	1.30	1.24
1	A	159	LYS	C-O	5.00	1.30	1.24
1	A	188	ARG	C-N	5.00	1.41	1.33

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	348	GLN	O-C-N	14.38	137.36	122.12
1	A	247	ASN	OD1-CG-ND2	13.01	135.61	122.60
1	B	306	CYS	O-C-N	12.88	135.34	122.07
1	B	157	ARG	NE-CZ-NH1	12.41	133.91	121.50
1	A	292	ARG	NE-CZ-NH1	-12.33	109.17	121.50
1	A	109	ARG	NE-CZ-NH1	11.92	133.42	121.50
1	A	298	GLY	O-C-N	11.71	135.04	122.28
1	A	261	GLY	O-C-N	11.58	134.69	122.65
1	B	211	LEU	O-C-N	11.42	138.13	122.37
1	A	205	ARG	NE-CZ-NH2	-11.32	109.01	119.20
1	A	307	MET	CA-C-O	11.10	132.19	120.42
1	B	348	GLN	CA-C-O	-11.08	108.81	120.55
1	A	215	ASN	O-C-N	11.04	131.40	121.36
1	A	109	ARG	NE-CZ-NH2	-10.72	109.55	119.20
1	A	305	GLY	O-C-N	10.63	133.51	122.24
1	A	123	ILE	O-C-N	10.42	131.98	121.87
1	A	349	ALA	O-C-N	10.09	133.65	122.15
1	B	24	ASP	CB-CA-C	10.08	124.78	109.56
1	B	208[A]	ARG	O-C-N	10.05	130.42	121.37
1	B	208[B]	ARG	O-C-N	10.05	130.42	121.37
1	B	260	PHE	CA-C-O	-10.03	110.16	121.19
1	B	260	PHE	O-C-N	9.94	135.09	122.87
1	A	239	GLY	CA-C-O	9.80	131.68	119.72
1	B	371	ALA	CA-C-O	9.80	132.97	120.81
1	B	154	ALA	O-C-N	9.79	132.50	122.12
1	B	153	ASP	CA-C-O	9.73	130.87	120.55
1	A	199	ALA	CA-C-O	-9.73	110.11	120.42
1	A	381	ASP	CA-CB-CG	9.55	122.15	112.60
1	A	81	ASP	CA-CB-CG	9.53	122.13	112.60
1	B	345	ASP	CA-CB-CG	9.51	122.11	112.60
1	A	181	GLU	O-C-N	9.40	130.03	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	185	ASN	OD1-CG-ND2	9.40	132.00	122.60
1	A	321	ARG	NE-CZ-NH2	-9.33	110.80	119.20
1	B	302	SER	O-C-N	9.18	132.62	122.15
1	A	189	GLY	CA-C-O	9.15	129.76	120.80
1	B	140	ARG	NH1-CZ-NH2	9.14	131.18	119.30
1	B	382	HIS	ND1-CG-CD2	9.06	115.16	106.10
1	B	169[A]	VAL	CA-C-O	-9.01	111.58	120.95
1	B	169[B]	VAL	CA-C-O	-9.01	111.58	120.95
1	A	249	GLN	OE1-CD-NE2	-9.00	113.60	122.60
1	B	347	LEU	O-C-N	-8.99	112.81	122.07
1	A	298	GLY	CA-C-O	-8.99	110.41	120.30
1	A	345	ASP	CA-CB-CG	8.98	121.58	112.60
1	B	205	ARG	NE-CZ-NH2	-8.98	111.12	119.20
1	B	374	ARG	NE-CZ-NH1	-8.97	112.53	121.50
1	B	31	ARG	NE-CZ-NH2	8.94	127.25	119.20
1	A	205	ARG	NH1-CZ-NH2	8.91	130.88	119.30
1	B	317	ALA	O-C-N	8.89	133.21	122.27
1	A	215	ASN	OD1-CG-ND2	8.79	131.39	122.60
1	A	213	GLY	O-C-N	8.71	134.03	122.70
1	B	171	SER	O-C-N	-8.65	112.95	122.12
1	B	313	LEU	O-C-N	8.62	132.31	122.22
1	B	245	ASP	N-CA-CB	-8.58	97.26	110.65
1	B	157	ARG	NE-CZ-NH2	-8.57	111.49	119.20
1	B	323	ASP	CA-C-O	8.51	126.02	119.46
1	A	292	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	B	321	ARG	NE-CZ-NH1	8.50	130.00	121.50
1	A	79	LEU	O-C-N	8.47	131.10	122.12
1	A	382	HIS	ND1-CE1-NE2	8.44	116.84	108.40
1	B	211	LEU	CA-C-O	-8.38	109.13	119.28
1	B	315	GLU	CA-C-O	8.37	129.61	120.82
1	A	113	ARG	NE-CZ-NH2	-8.35	111.68	119.20
1	A	24	ASP	CA-CB-CG	8.34	120.94	112.60
1	B	196	VAL	CA-C-O	-8.28	112.34	120.95
1	B	169[A]	VAL	O-C-N	8.28	129.90	121.87
1	B	169[B]	VAL	O-C-N	8.28	129.90	121.87
1	A	286	PHE	CA-C-O	8.26	129.44	120.43
1	A	315	GLU	CA-C-O	8.26	129.49	120.82
1	A	185	ASN	CA-C-O	-8.17	112.54	121.28
1	B	165	LEU	O-C-N	8.17	132.32	122.27
1	A	323	ASP	O-C-N	-8.17	114.37	121.31
1	A	320	PHE	O-C-N	8.16	130.47	122.07
1	A	261	GLY	CA-C-O	-8.13	110.77	119.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	THR	O-C-N	8.12	132.77	122.22
1	B	310	TYR	O-C-N	8.08	130.69	122.12
1	A	309	ASN	OD1-CG-ND2	8.08	130.68	122.60
1	B	135	VAL	O-C-N	8.07	132.19	122.83
1	A	203	ILE	CA-C-O	-8.04	111.96	120.57
1	A	368	ARG	NE-CZ-NH1	-8.04	113.46	121.50
1	A	23	ARG	O-C-N	-7.99	113.20	123.02
1	A	282	GLY	O-C-N	7.91	130.09	122.18
1	B	337	GLU	CG-CD-OE1	7.90	136.57	118.40
1	B	299	VAL	O-C-N	7.85	129.60	121.91
1	A	266	ARG	CD-NE-CZ	7.84	135.37	124.40
1	A	380	MET	O-C-N	7.81	130.39	122.12
1	A	127	VAL	O-C-N	7.80	129.87	121.83
1	B	170	THR	CA-C-O	-7.78	112.17	120.42
1	B	348	GLN	OE1-CD-NE2	-7.78	114.82	122.60
1	B	368	ARG	NE-CZ-NH1	-7.74	113.76	121.50
1	A	383	LEU	O-C-N	7.71	130.29	122.12
1	B	304	ALA	O-C-N	-7.70	113.96	122.12
1	B	196	VAL	CA-C-N	7.68	128.47	119.94
1	B	196	VAL	C-N-CA	7.68	128.47	119.94
1	B	266	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	A	197	GLY	O-C-N	-7.66	114.83	122.18
1	A	304	ALA	CA-C-O	7.65	128.66	120.55
1	A	90	THR	O-C-N	-7.60	115.28	123.26
1	B	23	ARG	O-C-N	-7.60	114.15	123.04
1	B	24	ASP	CA-CB-CG	7.53	120.13	112.60
1	B	220	HIS	O-C-N	-7.50	113.60	122.15
1	A	239	GLY	O-C-N	-7.49	114.32	122.41
1	B	262	ALA	O-C-N	-7.48	113.45	122.65
1	A	378	LEU	O-C-N	-7.46	114.21	122.12
1	A	24	ASP	OD1-CG-OD2	7.45	140.77	122.90
1	B	387	ARG	NE-CZ-NH1	7.44	128.94	121.50
1	B	205	ARG	NH1-CZ-NH2	7.43	128.96	119.30
1	A	11	PHE	O-C-N	-7.43	114.35	123.04
1	A	14	GLY	CA-C-O	-7.39	114.91	121.41
1	A	8	GLU	CB-CG-CD	7.39	125.16	112.60
1	B	321	ARG	O-C-N	7.37	131.33	122.27
1	B	102	GLY	CA-C-O	7.36	127.74	122.37
1	B	323	ASP	O-C-N	-7.36	115.06	121.31
1	B	266	ARG	NE-CZ-NH1	7.32	128.82	121.50
1	A	387	ARG	NE-CZ-NH1	7.31	128.81	121.50
1	B	115	ALA	O-C-N	7.29	129.84	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	GLU	O-C-N	-7.26	114.59	122.07
1	A	217	GLU	CG-CD-OE1	7.25	135.06	118.40
1	A	300	TRP	CA-C-O	7.23	128.29	119.97
1	A	368	ARG	NE-CZ-NH2	7.23	125.71	119.20
1	A	288	PHE	CA-C-O	7.22	129.56	121.40
1	B	327	GLN	CA-C-O	7.17	128.21	120.10
1	A	247	ASN	CA-C-O	7.13	128.36	120.94
1	A	61	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	302	SER	O-C-N	7.09	130.24	122.15
1	B	243	HIS	ND1-CE1-NE2	7.08	115.48	108.40
1	B	165	LEU	CA-C-O	-7.04	111.87	119.97
1	A	237	TRP	CA-C-O	-7.04	113.09	120.55
1	A	377	GLN	OE1-CD-NE2	-7.04	115.56	122.60
1	A	331	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	B	381	ASP	CA-CB-CG	7.00	119.60	112.60
1	B	181	GLU	CA-C-N	6.98	126.90	119.85
1	B	181	GLU	C-N-CA	6.98	126.90	119.85
1	A	349	ALA	CA-C-O	-6.96	113.04	120.42
1	A	201	ALA	CA-C-N	6.96	129.61	120.28
1	A	201	ALA	C-N-CA	6.96	129.61	120.28
1	A	148	ALA	O-C-N	6.96	131.75	122.43
1	B	332	ALA	O-C-N	6.94	130.34	122.22
1	A	259	ARG	O-C-N	-6.93	114.28	122.81
1	B	292	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	B	203	ILE	CA-C-O	-6.92	113.16	120.57
1	A	140	ARG	CA-C-O	-6.90	111.49	119.56
1	B	285	HIS	O-C-N	6.86	131.02	123.27
1	B	158[A]	MET	O-C-N	6.83	129.93	122.15
1	B	158[B]	MET	O-C-N	6.83	129.93	122.15
1	A	228	PHE	CA-C-O	-6.80	112.26	118.79
1	A	18	VAL	O-C-N	-6.79	114.32	122.06
1	A	123	ILE	CA-C-O	-6.76	113.91	120.95
1	A	382	HIS	CE1-NE2-CD2	-6.76	102.24	109.00
1	B	249	GLN	CA-C-O	6.74	128.83	120.54
1	B	374	ARG	CD-NE-CZ	-6.73	114.98	124.40
1	B	211	LEU	CA-C-N	-6.72	111.85	122.73
1	B	211	LEU	C-N-CA	-6.72	111.85	122.73
1	A	206	LEU	O-C-N	6.68	130.47	122.85
1	A	297	ASP	CA-C-O	6.68	127.63	120.55
1	B	350	LEU	O-C-N	-6.67	114.54	122.15
1	A	154	ALA	CA-C-O	-6.67	113.35	120.42
1	B	198	HIS	ND1-CE1-NE2	6.67	115.07	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	TRP	O-C-N	-6.66	114.08	122.27
1	B	162	PHE	O-C-N	6.66	130.46	122.27
1	B	259	ARG	CA-C-O	6.64	128.59	121.55
1	B	371	ALA	N-CA-C	6.61	120.70	112.24
1	A	366	ALA	CA-C-O	-6.59	112.39	119.97
1	A	222	GLN	CA-C-O	-6.58	112.41	119.97
1	A	116	LEU	CA-C-O	-6.57	113.45	120.42
1	B	243	HIS	CE1-NE2-CD2	-6.56	102.44	109.00
1	B	100	LYS	O-C-N	-6.56	113.86	122.39
1	B	182	PRO	N-CA-CB	6.55	109.42	103.33
1	A	74	ARG	CA-C-O	6.55	127.49	120.55
1	A	125	LEU	O-C-N	-6.55	114.69	122.15
1	B	382	HIS	CG-CD2-NE2	-6.54	100.66	107.20
1	B	111	VAL	CA-C-O	-6.53	113.92	120.85
1	A	201	ALA	O-C-N	-6.52	114.72	122.15
1	A	212	TYR	CB-CG-CD1	6.52	130.57	120.80
1	B	221	GLU	O-C-N	6.50	129.56	122.15
1	A	295	ASP	CB-CG-OD1	6.48	133.29	118.40
1	A	313	LEU	O-C-N	6.47	129.79	122.22
1	A	188	ARG	CA-C-O	6.46	129.35	121.72
1	B	96	HIS	CE1-NE2-CD2	6.46	115.46	109.00
1	A	348	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	B	321	ARG	CA-C-O	-6.44	112.56	119.97
1	B	319	ALA	O-C-N	-6.44	115.29	122.12
1	A	292	ARG	O-C-N	6.43	131.82	122.43
1	B	117	ARG	NE-CZ-NH1	-6.42	115.08	121.50
1	B	109	ARG	O-C-N	-6.42	114.83	122.15
1	B	132[A]	GLU	CA-C-O	6.42	126.20	119.14
1	B	132[B]	GLU	CA-C-O	6.42	126.20	119.14
1	B	94	PHE	CA-C-O	-6.41	111.16	118.47
1	A	276	GLU	CA-C-O	-6.41	113.63	120.42
1	B	375	LEU	CA-C-O	6.39	127.53	120.82
1	A	131	ALA	CA-C-O	-6.38	114.02	121.16
1	A	127	VAL	CA-C-O	-6.37	114.09	120.85
1	B	151	VAL	O-C-N	6.36	128.99	121.80
1	B	140	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	B	362	VAL	O-C-N	6.36	128.29	121.87
1	B	24	ASP	O-C-N	6.36	126.72	121.32
1	A	387	ARG	NH1-CZ-NH2	-6.34	111.06	119.30
1	B	292	ARG	NE-CZ-NH1	-6.33	115.17	121.50
1	B	329	ALA	O-C-N	6.31	130.03	122.27
1	A	42	ARG	CA-C-O	6.31	127.11	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160[A]	GLU	O-C-N	-6.31	115.44	122.12
1	B	160[B]	GLU	O-C-N	-6.31	115.44	122.12
1	A	189	GLY	N-CA-C	6.30	120.52	112.83
1	B	325	GLU	O-C-N	6.30	130.02	122.27
1	A	213	GLY	CA-C-N	-6.30	112.09	122.67
1	A	213	GLY	C-N-CA	-6.30	112.09	122.67
1	A	290	PRO	CA-C-N	-6.29	113.47	119.89
1	A	290	PRO	C-N-CA	-6.29	113.47	119.89
1	A	120	ILE	CA-C-O	-6.28	114.42	120.95
1	A	311	LEU	CA-C-O	6.28	127.08	120.42
1	A	21	GLU	CA-C-O	-6.27	111.09	119.11
1	B	255	ASP	CA-CB-CG	6.27	118.87	112.60
1	B	8	GLU	CB-CG-CD	6.26	123.24	112.60
1	B	232	ILE	CA-C-O	-6.26	113.71	120.47
1	B	153	ASP	O-C-N	-6.25	115.49	122.12
1	B	364	ALA	CA-C-O	6.23	127.15	120.55
1	A	230	HIS	CA-C-N	6.23	126.89	119.98
1	A	230	HIS	C-N-CA	6.23	126.89	119.98
1	B	8	GLU	N-CA-C	6.21	119.96	112.38
1	B	302	SER	CA-C-O	-6.21	113.83	120.42
1	B	176	ILE	O-C-N	-6.21	116.05	122.63
1	A	38	GLU	CA-C-O	6.21	127.13	120.55
1	A	107	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	A	253[A]	LYS	CA-C-O	-6.21	114.49	120.94
1	A	253[B]	LYS	CA-C-O	-6.21	114.49	120.94
1	B	376	ASP	CA-CB-CG	-6.21	106.39	112.60
1	A	380	MET	CA-C-O	-6.21	113.97	120.55
1	A	146	GLY	CA-C-O	-6.20	113.45	120.09
1	A	357	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	308	ARG	O-C-N	-6.20	115.68	122.07
1	B	266	ARG	N-CA-CB	6.19	119.22	110.12
1	B	306	CYS	CA-C-O	-6.18	114.33	120.82
1	A	185	ASN	O-C-N	6.17	129.46	123.29
1	A	112	ARG	O-C-N	6.17	128.66	122.12
1	B	100	LYS	CA-C-O	6.17	126.95	119.49
1	B	140	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	B	265	LEU	CA-C-O	-6.16	113.89	120.42
1	B	271	LEU	CA-C-O	-6.14	114.38	120.70
1	B	225	GLY	O-C-N	6.14	130.08	122.41
1	B	304	ALA	CA-C-O	6.13	127.05	120.55
1	A	234	GLN	CA-C-O	-6.12	113.93	120.42
1	A	110	ASP	CA-CB-CG	6.12	118.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	ALA	CA-C-O	-6.11	114.41	120.70
1	B	157	ARG	CA-C-O	6.11	127.02	120.55
1	B	378	LEU	CA-C-O	6.10	126.88	120.42
1	A	31	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
1	A	130	GLY	CA-C-N	-6.09	112.22	120.87
1	A	130	GLY	C-N-CA	-6.09	112.22	120.87
1	B	347	LEU	CA-C-O	6.09	127.21	120.82
1	B	55	ASP	CA-CB-CG	6.07	118.67	112.60
1	B	247	ASN	CA-C-O	6.07	127.25	120.94
1	A	302	SER	N-CA-CB	-6.07	101.18	110.16
1	A	273	ASP	O-C-N	6.07	128.40	122.09
1	B	138	GLY	O-C-N	6.03	130.53	122.70
1	A	259	ARG	CA-C-O	6.02	127.93	121.55
1	A	203	ILE	O-C-N	6.02	127.95	121.87
1	A	307	MET	N-CA-C	6.02	117.92	111.36
1	B	327	GLN	O-C-N	-6.01	115.18	122.22
1	A	369	GLY	CA-C-O	-6.01	114.86	121.71
1	A	208	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	B	239	GLY	CA-C-O	5.99	127.03	119.72
1	B	374	ARG	CA-C-O	5.99	126.89	120.55
1	B	177	ARG	CA-C-O	-5.97	114.48	121.46
1	B	167[A]	GLU	O-C-N	-5.96	115.81	122.12
1	B	167[B]	GLU	O-C-N	-5.96	115.81	122.12
1	B	91	THR	CA-C-N	-5.95	113.66	122.41
1	B	91	THR	C-N-CA	-5.95	113.66	122.41
1	B	184	PRO	O-C-N	5.95	130.68	122.64
1	B	269	PHE	CA-C-O	-5.95	114.58	120.82
1	B	111	VAL	O-C-N	5.93	127.94	121.83
1	B	137	TRP	O-C-N	5.93	130.95	123.12
1	B	151	VAL	CA-C-O	-5.91	114.09	120.47
1	A	50	GLY	O-C-N	5.90	130.75	123.61
1	B	287	ASP	O-C-N	5.89	131.59	122.87
1	A	139	GLY	CA-C-O	-5.87	113.84	120.30
1	B	118	LYS	O-C-N	5.87	128.84	122.15
1	B	154	ALA	CA-C-O	-5.86	114.34	120.55
1	A	204	GLU	CA-C-O	-5.86	111.44	119.05
1	B	341	PRO	O-C-N	-5.86	115.45	122.89
1	B	105	THR	CA-C-O	-5.85	112.87	119.95
1	A	19	GLY	O-C-N	5.85	130.98	122.26
1	A	205	ARG	CG-CD-NE	-5.85	99.13	112.00
1	B	354	ARG	CA-C-O	-5.84	112.20	119.38
1	A	178	PHE	CA-C-O	5.83	128.16	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	PRO	CA-C-N	-5.83	111.26	120.47
1	B	97	PRO	C-N-CA	-5.83	111.26	120.47
1	A	296	PHE	O-C-N	-5.82	115.41	122.22
1	A	83	GLY	O-C-N	5.79	129.22	122.45
1	A	76	ARG	O-C-N	5.77	128.97	122.22
1	B	54	HIS	CE1-NE2-CD2	-5.77	103.23	109.00
1	A	309	ASN	CA-C-N	-5.74	112.97	120.44
1	A	309	ASN	C-N-CA	-5.74	112.97	120.44
1	B	256	GLN	N-CA-C	5.74	119.46	112.23
1	A	72	VAL	O-C-N	5.73	127.74	121.83
1	A	91	THR	CA-C-O	-5.73	114.63	120.71
1	B	195	THR	CA-C-O	-5.73	115.09	121.51
1	A	255	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	308	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	309	ASN	O-C-N	5.71	129.29	122.27
1	A	148	ALA	CA-C-O	-5.70	112.36	119.38
1	B	287	ASP	CA-C-N	-5.70	112.97	122.21
1	B	287	ASP	C-N-CA	-5.70	112.97	122.21
1	A	98	VAL	CA-C-O	-5.70	114.47	120.57
1	A	305	GLY	CA-C-N	-5.70	112.85	120.54
1	A	305	GLY	C-N-CA	-5.70	112.85	120.54
1	A	92	ASN	O-C-N	5.69	130.22	122.82
1	B	220	HIS	CA-C-O	5.69	126.45	120.42
1	A	335	LEU	O-C-N	5.68	129.25	122.27
1	B	169[A]	VAL	N-CA-CB	-5.66	102.84	110.54
1	B	169[B]	VAL	N-CA-CB	-5.66	102.84	110.54
1	A	42	ARG	CD-NE-CZ	5.66	132.32	124.40
1	A	77	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	151	VAL	CA-C-O	-5.65	114.86	120.85
1	B	299	VAL	CA-C-O	-5.63	115.20	121.17
1	A	29	ALA	O-C-N	5.63	129.79	122.87
1	A	208	ARG	NH1-CZ-NH2	5.63	126.61	119.30
1	A	366	ALA	O-C-N	5.62	129.19	122.27
1	B	285	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	B	115	ALA	CA-C-N	-5.62	112.32	120.29
1	B	115	ALA	C-N-CA	-5.62	112.32	120.29
1	B	163	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	54	HIS	CG-CD2-NE2	5.61	112.81	107.20
1	B	119	THR	CA-C-N	-5.61	112.78	120.46
1	B	119	THR	C-N-CA	-5.61	112.78	120.46
1	A	88	MET	O-C-N	-5.60	117.00	123.33
1	B	196	VAL	N-CA-C	-5.60	104.91	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	TYR	CA-C-O	5.59	126.27	120.40
1	A	318	ALA	CA-C-O	5.58	126.46	120.55
1	B	253[A]	LYS	CA-C-O	-5.58	115.14	120.94
1	B	253[B]	LYS	CA-C-O	-5.58	115.14	120.94
1	B	294	GLU	N-CA-C	5.57	119.18	110.32
1	B	309	ASN	CA-C-N	-5.56	112.84	120.28
1	B	309	ASN	C-N-CA	-5.56	112.84	120.28
1	B	335	LEU	N-CA-C	-5.55	105.38	111.82
1	A	162	PHE	O-C-N	5.55	128.48	122.15
1	A	301	ALA	O-C-N	5.54	127.99	122.12
1	B	118	LYS	CA-C-O	-5.54	114.55	120.42
1	A	38	GLU	CA-CB-CG	5.54	125.17	114.10
1	B	297	ASP	CA-C-N	5.53	126.08	120.00
1	B	297	ASP	C-N-CA	5.53	126.08	120.00
1	B	31	ARG	O-C-N	5.52	130.02	123.24
1	A	90	THR	CA-C-O	5.51	127.22	121.38
1	A	373	GLU	CG-CD-OE1	5.51	131.09	118.40
1	B	331	ARG	CA-C-O	5.51	126.26	120.42
1	A	286	PHE	CB-CG-CD1	5.51	130.07	120.70
1	B	290	PRO	N-CA-C	-5.51	103.98	110.70
1	A	331	ARG	NH1-CZ-NH2	5.50	126.45	119.30
1	B	191	ILE	CA-C-O	5.49	127.21	120.84
1	A	307	MET	O-C-N	-5.49	115.90	122.15
1	A	282	GLY	CA-C-O	-5.47	116.75	122.38
1	B	198	HIS	CE1-NE2-CD2	-5.47	103.53	109.00
1	B	113	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	B	21	GLU	CA-C-O	-5.46	111.97	119.12
1	A	202	PHE	O-C-N	5.45	127.90	122.12
1	A	373	GLU	CA-C-O	-5.45	114.64	120.42
1	A	122	ASN	OD1-CG-ND2	5.45	128.05	122.60
1	B	86	VAL	CA-C-N	5.44	124.96	119.19
1	B	86	VAL	C-N-CA	5.44	124.96	119.19
1	B	10[A]	ARG	CA-C-N	-5.43	114.53	122.19
1	B	10[A]	ARG	C-N-CA	-5.43	114.53	122.19
1	B	10[B]	ARG	CA-C-N	-5.43	114.53	122.19
1	B	10[B]	ARG	C-N-CA	-5.43	114.53	122.19
1	B	326	VAL	CA-C-N	-5.43	112.47	120.28
1	B	326	VAL	C-N-CA	-5.43	112.47	120.28
1	A	255	ASP	O-C-N	5.42	130.09	122.77
1	A	249	GLN	CG-CD-OE1	5.42	131.64	120.80
1	B	340	ARG	CA-C-O	5.42	125.23	120.19
1	A	375	LEU	CA-C-O	5.42	126.30	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	GLY	O-C-N	-5.42	117.26	122.84
1	B	109	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	B	218	VAL	O-C-N	5.41	129.34	122.57
1	A	272	VAL	O-C-N	-5.41	116.26	121.83
1	A	376	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	339	ALA	CA-C-O	-5.40	112.75	119.28
1	A	163	ASP	CA-C-O	-5.39	114.70	120.42
1	A	224	ALA	O-C-N	-5.39	115.88	122.34
1	B	312	ILE	CA-C-O	5.38	126.88	121.17
1	A	19	GLY	CA-C-N	-5.38	113.49	121.24
1	A	19	GLY	C-N-CA	-5.38	113.49	121.24
1	B	344	ALA	CA-C-O	-5.37	112.78	119.38
1	B	110	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	119	THR	O-C-N	5.36	127.80	122.12
1	B	57	ASP	CA-CB-CG	5.35	117.95	112.60
1	B	149	LYS	O-C-N	-5.35	116.43	123.28
1	B	306	CYS	CA-C-N	-5.34	112.71	120.29
1	B	306	CYS	C-N-CA	-5.34	112.71	120.29
1	A	376	ASP	O-C-N	5.33	128.82	122.27
1	A	247	ASN	N-CA-C	-5.33	100.59	107.73
1	B	313	LEU	CA-C-O	-5.32	114.09	120.10
1	B	137	TRP	CA-C-O	-5.30	114.83	120.40
1	B	107	ASN	CA-C-O	-5.30	114.11	120.10
1	B	344	ALA	N-CA-C	-5.30	106.07	112.54
1	B	310	TYR	CA-C-O	-5.30	114.93	120.55
1	A	347	LEU	O-C-N	-5.30	116.61	122.07
1	A	280	TYR	CB-CG-CD1	5.29	128.74	120.80
1	B	223	MET	O-C-N	-5.29	115.51	122.39
1	A	248	GLY	O-C-N	5.28	128.23	123.42
1	B	317	ALA	CA-C-N	-5.28	112.79	120.29
1	B	317	ALA	C-N-CA	-5.28	112.79	120.29
1	B	43	LEU	O-C-N	5.27	128.16	122.15
1	A	161	ALA	CA-C-O	-5.27	115.29	120.82
1	B	158[A]	MET	CA-C-O	-5.27	114.83	120.42
1	B	158[B]	MET	CA-C-O	-5.27	114.83	120.42
1	A	315	GLU	N-CA-C	5.26	116.70	111.07
1	A	270	TRP	CD2-CE2-CZ2	5.26	127.66	122.40
1	A	166	GLY	CA-C-O	-5.26	115.09	120.66
1	B	365	ALA	O-C-N	5.25	128.13	122.15
1	A	208	ARG	O-C-N	5.25	126.09	121.37
1	B	103	GLY	N-CA-C	-5.24	105.44	110.21
1	B	205	ARG	CG-CD-NE	-5.24	100.48	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	PRO	O-C-N	5.23	127.63	121.46
1	B	253[A]	LYS	CG-CD-CE	5.22	123.31	111.30
1	B	253[B]	LYS	CG-CD-CE	5.22	123.31	111.30
1	B	349	ALA	O-C-N	5.22	127.65	122.12
1	B	213	GLY	O-C-N	5.21	129.48	122.70
1	A	212	TYR	CA-C-O	5.21	126.65	120.66
1	B	276	GLU	CA-C-O	-5.21	113.64	119.79
1	B	234	GLN	CA-C-O	-5.21	114.90	120.42
1	A	373	GLU	O-C-N	5.21	128.09	122.15
1	B	285	HIS	CA-C-N	-5.20	115.55	122.72
1	B	285	HIS	C-N-CA	-5.20	115.55	122.72
1	A	41	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	B	167[A]	GLU	CA-C-O	5.19	126.05	120.55
1	B	167[B]	GLU	CA-C-O	5.19	126.05	120.55
1	A	314	LYS	CA-C-O	5.18	126.04	120.55
1	B	157	ARG	N-CA-C	5.18	116.93	111.28
1	A	31	ARG	NE-CZ-NH1	5.18	126.68	121.50
1	A	362	VAL	O-C-N	5.18	127.65	121.80
1	B	148	ALA	O-C-N	5.18	129.37	122.43
1	A	263	GLY	O-C-N	-5.17	116.85	122.90
1	A	321	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	B	148	ALA	CA-C-N	-5.17	114.74	122.39
1	B	148	ALA	C-N-CA	-5.17	114.74	122.39
1	A	16	TRP	CD2-CE2-CZ2	5.17	127.57	122.40
1	B	177	ARG	O-C-N	5.15	130.02	123.11
1	A	212	TYR	CB-CG-CD2	-5.15	113.08	120.80
1	B	196	VAL	N-CA-CB	-5.14	103.54	110.54
1	B	261	GLY	O-C-N	5.14	128.00	122.65
1	A	265	LEU	O-C-N	-5.13	116.30	122.15
1	B	27	GLY	CA-C-O	-5.13	116.44	121.06
1	B	387	ARG	NE-CZ-NH2	-5.13	114.58	119.20
1	A	78	ALA	CA-C-O	5.13	125.86	120.42
1	A	276	GLU	CG-CD-OE2	5.13	130.19	118.40
1	A	217	GLU	O-C-N	-5.12	117.21	123.30
1	B	337	GLU	OE1-CD-OE2	-5.12	110.62	122.90
1	B	154	ALA	CA-C-N	-5.11	112.54	120.31
1	B	154	ALA	C-N-CA	-5.11	112.54	120.31
1	B	231	GLY	CA-C-O	-5.11	115.25	120.66
1	B	243	HIS	CA-C-N	-5.10	115.03	122.58
1	B	243	HIS	C-N-CA	-5.10	115.03	122.58
1	B	222	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	B	116	LEU	O-C-N	-5.09	116.35	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	ARG	NH1-CZ-NH2	5.09	125.91	119.30
1	B	96	HIS	ND1-CE1-NE2	-5.08	103.32	108.40
1	B	320	PHE	O-C-N	5.08	127.37	122.09
1	B	326	VAL	O-C-N	5.08	127.06	121.83
1	A	152	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	349	ALA	CA-C-N	-5.07	113.48	120.28
1	A	349	ALA	C-N-CA	-5.07	113.48	120.28
1	A	190	ASP	CA-CB-CG	-5.07	107.53	112.60
1	A	311	LEU	N-CA-C	5.07	116.89	111.36
1	A	335	LEU	CA-C-O	-5.07	114.14	119.97
1	B	249	GLN	CA-C-N	-5.06	115.28	122.77
1	B	249	GLN	C-N-CA	-5.06	115.28	122.77
1	A	162	PHE	CA-C-N	-5.06	113.10	120.29
1	A	162	PHE	C-N-CA	-5.06	113.10	120.29
1	A	320	PHE	CA-C-O	-5.06	115.51	120.82
1	A	321	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	B	135	VAL	CA-C-N	-5.04	115.88	122.99
1	B	135	VAL	C-N-CA	-5.04	115.88	122.99
1	A	277	SER	CA-CB-OG	-5.04	101.02	111.10
1	A	252	ILE	O-C-N	-5.04	115.58	122.59
1	A	344	ALA	N-CA-C	-5.04	106.39	112.54
1	A	220	HIS	O-C-N	-5.04	116.07	122.27
1	B	382	HIS	N-CA-C	5.04	116.85	111.36
1	A	47	GLY	O-C-N	5.03	128.09	122.50
1	B	97	PRO	O-C-N	5.03	128.98	122.24
1	B	301	ALA	O-C-N	-5.03	116.79	122.12
1	A	306	CYS	O-C-N	5.02	127.31	122.09
1	A	268	ALA	CA-C-O	-5.02	115.10	120.42
1	B	374	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	196	VAL	O-C-N	-5.01	117.01	121.87
1	A	320	PHE	CA-C-N	-5.01	112.36	120.72
1	A	320	PHE	C-N-CA	-5.01	112.36	120.72

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	3060	0	2925	34	0
1	B	3095	0	2955	41	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	14	0	0
4	B	8	0	14	0	0
5	A	9	0	14	1	0
5	B	9	0	14	0	0
6	A	8	0	12	0	0
7	B	8	0	14	5	0
8	A	474	0	0	11	1
8	B	437	0	0	9	0
All	All	7120	0	5962	74	1

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 6.

All (74) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132[B]:GLU:HG3	8:B:2187:HOH:O	1.28	1.26
1:A:10[B]:ARG:HH21	1:A:284:ARG:NH1	1.35	1.24
1:A:10[B]:ARG:NH2	1:A:284:ARG:NH1	1.86	1.23
1:A:10[B]:ARG:HH21	1:A:284:ARG:CZ	1.64	1.09
1:B:132[B]:GLU:OE2	8:B:2188:HOH:O	1.77	1.00
8:A:2036:HOH:O	1:B:25:PRO:HB3	1.63	0.96
1:B:35:ASP:HB3	1:B:38[A]:GLU:HG3	1.48	0.94
1:A:160[A]:GLU:OE2	8:A:2253:HOH:O	1.85	0.94
1:B:61:PHE:CE2	8:B:2154:HOH:O	2.21	0.94
1:A:331:ARG:HB3	7:B:396:MPD:H13	1.51	0.93
1:B:96:HIS:HD2	1:B:98:VAL:H	1.09	0.92
1:A:10[B]:ARG:NH2	1:A:284:ARG:CZ	2.28	0.90
1:A:42:ARG:HG2	8:A:2064:HOH:O	1.72	0.86
1:A:61:PHE:CE2	8:A:2191:HOH:O	2.32	0.82
1:A:42:ARG:HD2	8:A:2078:HOH:O	1.85	0.77
8:A:2036:HOH:O	1:B:25:PRO:CB	2.25	0.75
1:B:61:PHE:HE2	8:B:2154:HOH:O	1.63	0.75
1:A:10[B]:ARG:NH2	1:A:284:ARG:HH12	1.83	0.74
1:B:96:HIS:CD2	1:B:98:VAL:H	2.00	0.74
1:A:2:ASN:N	8:A:2001:HOH:O	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ASP:OD2	7:B:396:MPD:CM	2.41	0.68
1:A:61:PHE:CD2	8:A:2096:HOH:O	2.47	0.67
1:A:337:GLU:OE2	7:B:396:MPD:H51	1.95	0.66
1:B:10[B]:ARG:NH2	1:B:284:ARG:NH1	2.44	0.66
1:B:132[A]:GLU:HG3	8:B:2187:HOH:O	1.96	0.65
1:A:24:ASP:HB2	1:A:25:PRO:CD	2.29	0.62
1:A:10[B]:ARG:CZ	1:A:284:ARG:NH1	2.63	0.61
1:A:336:ASP:OD2	7:B:396:MPD:HM1	2.02	0.59
1:B:61:PHE:CD2	8:B:2075:HOH:O	2.52	0.59
1:A:61:PHE:HE2	8:A:2191:HOH:O	1.77	0.59
1:B:87:PRO:O	1:B:132[B]:GLU:OE2	2.20	0.59
1:B:10[B]:ARG:HH21	1:B:284:ARG:CZ	2.15	0.58
1:B:132[B]:GLU:CD	8:B:2188:HOH:O	2.38	0.57
1:B:32:ARG:HG2	1:B:296:PHE:HE2	1.72	0.55
1:A:336:ASP:OD2	7:B:396:MPD:HM3	2.06	0.55
1:A:42:ARG:NH2	8:A:2072:HOH:O	2.20	0.54
1:B:328[B]:GLU:OE1	1:B:331:ARG:NH2	2.28	0.54
1:B:10[B]:ARG:HH21	1:B:284:ARG:NH1	2.07	0.52
1:B:41[B]:ARG:HH12	1:B:81:ASP:HB2	1.77	0.50
1:B:132[A]:GLU:OE2	8:B:2187:HOH:O	2.18	0.50
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.94	0.50
1:A:24:ASP:CB	1:A:25:PRO:CD	2.89	0.49
1:B:32:ARG:HG2	1:B:296:PHE:CE2	2.47	0.49
1:B:96:HIS:CD2	1:B:97:PRO:HD2	2.47	0.49
1:B:10[B]:ARG:NH2	1:B:284:ARG:CZ	2.75	0.49
1:A:42:ARG:NE	8:A:2072:HOH:O	2.38	0.48
1:B:8:GLU:H	1:B:8:GLU:CD	2.21	0.48
1:B:170:THR:HG21	1:B:208[A]:ARG:CZ	2.44	0.48
5:A:395:MQD:H4	5:A:395:MQD:HMC1	1.62	0.47
1:A:158[B]:MET:SD	1:A:193:LEU:HD11	2.55	0.46
1:B:24:ASP:HB2	1:B:25:PRO:HD2	1.96	0.46
1:B:158[B]:MET:SD	1:B:193:LEU:HD11	2.55	0.46
1:A:97:PRO:HB3	1:B:30:THR:HG22	1.98	0.46
1:A:35:ASP:HB3	1:A:38:GLU:HG3	1.98	0.46
1:B:132[A]:GLU:CG	8:B:2187:HOH:O	2.61	0.46
1:B:24:ASP:HB2	1:B:25:PRO:CD	2.45	0.45
1:B:170:THR:HG21	1:B:208[A]:ARG:NH1	2.32	0.45
1:A:252:ILE:HG22	1:B:252:ILE:HG22	1.97	0.45
1:A:24:ASP:HB2	1:A:25:PRO:HD3	1.99	0.45
1:A:25:PRO:HB2	1:A:26:PHE:CD1	2.53	0.44
1:B:34:LEU:HD21	1:B:296:PHE:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:HIS:O	1:A:55:ASP:C	2.62	0.43
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.96	0.43
1:B:101:ASP:O	1:B:101:ASP:CG	2.62	0.42
1:A:186:GLU:HA	1:A:187:PRO:HA	1.95	0.42
1:B:157:ARG:HH21	1:B:160[A]:GLU:CD	2.25	0.41
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.55	0.41
1:A:227:ASN:OD1	1:A:229:PRO:HD2	2.21	0.41
1:B:8:GLU:CD	1:B:8:GLU:N	2.79	0.41
1:B:96:HIS:CG	1:B:97:PRO:HD2	2.56	0.40
1:A:167:GLU:O	1:A:171:SER:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2136:HOH:O	8:A:2233:HOH:O[2_665]	2.08	0.12

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/304 (101%)	303 (99%)	4 (1%)	61	35
1	B	315/304 (104%)	311 (99%)	4 (1%)	61	35
All	All	622/608 (102%)	614 (99%)	8 (1%)	68	35

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10[A]	ARG
1	A	10[B]	ARG
1	A	91	THR
1	A	245	ASP
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	66	SER
1	B	245	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	96	HIS
1	B	172	GLN

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	MRD	A	394	-	7,7,7	0.66	0	9,10,10	0.98	0
5	MQD	B	395	3	7,8,8	0.96	1 (14%)	6,11,11	1.10	0
7	MPD	B	396	-	7,7,7	0.94	0	9,10,10	2.25	4 (44%)
6	TRS	A	396	-	7,7,7	0.99	0	9,9,9	1.61	2 (22%)
5	MQD	A	395	3	7,8,8	0.74	0	6,11,11	0.96	0
4	MRD	B	394	-	7,7,7	0.47	0	9,10,10	0.88	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRD	A	394	-	-	2/5/5/5	-
5	MQD	B	395	3	-	1/8/8/8	-
7	MPD	B	396	-	-	3/5/5/5	-
6	TRS	A	396	-	-	0/9/9/9	-
5	MQD	A	395	3	-	5/8/8/8	-
4	MRD	B	394	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	395	MQD	C1-C2	2.05	1.54	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	396	MPD	O2-C2-C1	4.08	120.72	107.99
6	A	396	TRS	C3-C-N	3.37	116.78	108.17
7	B	396	MPD	O2-C2-CM	3.22	118.03	107.99
6	A	396	TRS	C3-C-C1	-2.82	103.14	110.66
7	B	396	MPD	C1-C2-C3	-2.60	98.96	110.20
7	B	396	MPD	O4-C4-C3	-2.20	102.58	111.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	395	MQD	C1-C2-CM-O6

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Mol	Chain	Res	Type	Atoms
5	A	395	MQD	O2-C2-CM-O6
4	B	394	MRD	O2-C2-C3-C4
5	A	395	MQD	C3-C2-CM-O6
5	A	395	MQD	C1-C2-C3-C4
5	B	395	MQD	C1-C2-C3-C4
4	A	394	MRD	O2-C2-C3-C4
7	B	396	MPD	O2-C2-C3-C4
4	A	394	MRD	CM-C2-C3-C4
7	B	396	MPD	C1-C2-C3-C4
7	B	396	MPD	CM-C2-C3-C4
5	A	395	MQD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	396	MPD	5	0
5	A	395	MQD	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	387/388 (99%)	-0.61	2 (0%) 87 89	8, 13, 24, 34	4 (1%)
1	B	386/388 (99%)	-0.55	2 (0%) 87 89	8, 14, 27, 44	12 (3%)
All	All	773/776 (99%)	-0.58	4 (0%) 87 89	8, 13, 26, 44	16 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PRO	3.4
1	A	25	PRO	3.3
1	B	296	PHE	3.2
1	A	2	ASN	2.1

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
7	MPD	B	396	8/8	0.80	0.27	5,20,28,33	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MRD	A	394	8/8	0.83	0.14	24,31,38,38	0
6	TRS	A	396	8/8	0.87	0.11	28,30,32,35	0
4	MRD	B	394	8/8	0.92	0.09	21,27,32,34	0
5	MQD	A	395	9/9	0.93	0.10	18,25,27,27	0
5	MQD	B	395	9/9	0.94	0.09	21,24,25,29	0
3	MG	A	392	1/1	0.99	0.03	11,11,11,11	0
3	MG	B	392	1/1	0.99	0.04	12,12,12,12	0
2	MN	A	390	1/1	1.00	0.01	14,14,14,14	0
2	MN	B	390	1/1	1.00	0.03	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.