



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:13 AM UTC

PDB ID : 1GQO / pdb_00001gqo
Title : Type II Dehydroquinase from Bacillus subtilis
Authors : Robinson, D.A.; Roszak, A.W.; Coggins, J.R.; Lapthorn, A.J.
Deposited on : 2001-11-28
Resolution : 2.10 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

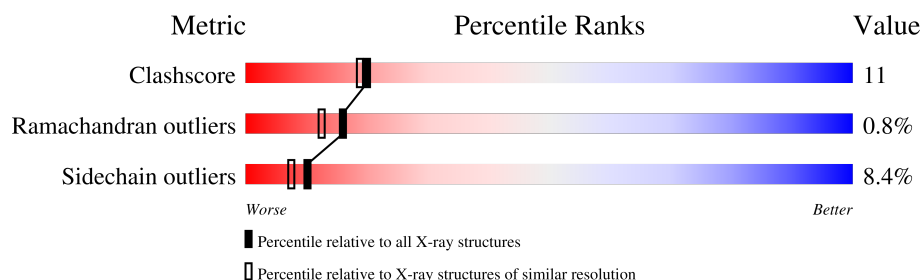
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

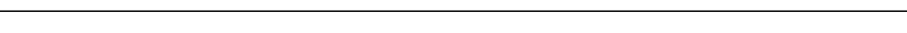
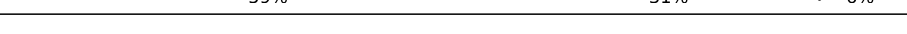
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	56% 34% 8% ..
1	B	143	57% 32% 10% .
1	C	143	63% 30% 6% .
1	D	143	59% 34% . ..
1	E	143	59% 29% 10% ..
1	F	143	68% 26% 5% ..
1	G	143	55% 38% 5% ..
1	H	143	54% 32% 11% ..

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Mol	Chain	Length	Quality of chain
1	I	143	 55% 34% 8% ..
1	J	143	 61% 29% 9% ..
1	K	143	 55% 36% 5% ..
1	L	143	 55% 33% 9% ..
1	M	143	 59% 31% 8% ..
1	N	143	 57% 31% 7% ..
1	O	143	 59% 35% ..
1	P	143	 64% 25% 8% ..
1	Q	143	 64% 30% ..
1	R	143	 59% 31% 8% ..
1	S	143	 60% 31% 7% ..
1	T	143	 64% 29% 6% ..
1	U	143	 59% 31% 8% ..
1	V	143	 66% 23% 5% 5%
1	X	143	 59% 31% 6%
1	Y	143	 57% 31% 10% ..

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
2	GOL	C	151	-	-	X	-
2	GOL	D	151	-	-	X	-
2	GOL	D	152	-	X	-	-
2	GOL	F	150	-	X	-	-
2	GOL	G	151	-	-	X	-
2	GOL	I	150	-	X	-	-
2	GOL	K	152	-	-	X	-
2	GOL	L	150	-	X	-	-
2	GOL	L	151	-	-	X	-
2	GOL	O	150	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	O	151	-	-	X	-
2	GOL	O	152	-	-	X	-
2	GOL	P	151	-	-	X	-
2	GOL	Q	151	-	-	X	-
2	GOL	R	150	-	X	-	-
2	GOL	R	151	-	-	X	-
2	GOL	S	150	-	X	-	-
2	GOL	S	151	-	-	X	-
2	GOL	S	152	-	-	X	-
2	GOL	U	151	-	-	X	-
2	GOL	Y	151	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28764 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 DEHYDROQUINASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	0	0	1
			1094	696	190	208			
1	B	143	Total	C	N	O	0	0	0
			1105	705	191	209			
1	C	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	D	142	Total	C	N	O	0	1	1
			1094	696	191	207			
1	E	142	Total	C	N	O	0	2	1
			1108	707	190	211			
1	F	142	Total	C	N	O	0	3	1
			1107	706	191	210			
1	G	142	Total	C	N	O	0	2	1
			1101	702	191	208			
1	H	142	Total	C	N	O	0	0	1
			1096	700	190	206			
1	I	142	Total	C	N	O	0	0	1
			1090	694	190	206			
1	J	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	K	137	Total	C	N	O	0	0	1
			1051	667	185	199			
1	L	142	Total	C	N	O	0	1	1
			1085	689	191	205			
1	M	142	Total	C	N	O	0	1	1
			1098	698	193	207			
1	N	133	Total	C	N	O	0	0	1
			1028	656	178	194			
1	O	142	Total	C	N	O	0	0	1
			1096	697	193	206			
1	P	142	Total	C	N	O	0	0	1
			1099	703	190	206			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	0	0	1
			1109	708	193	208			
1	R	142	Total	C	N	O	0	1	1
			1094	696	190	208			
1	S	142	Total	C	N	O	0	0	1
			1108	707	193	208			
1	T	142	Total	C	N	O	0	1	1
			1104	705	190	209			
1	U	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	V	136	Total	C	N	O	0	0	1
			1056	674	184	198			
1	X	134	Total	C	N	O	0	0	1
			1034	659	179	196			
1	Y	142	Total	C	N	O	0	0	1
			1096	700	190	206			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			5	3	2		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			5	3	2		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total 6	C 3	O 3	0	0
2	P	1	Total 6	C 3	O 3	0	0
2	P	1	Total 6	C 3	O 3	0	0
2	Q	1	Total 6	C 3	O 3	0	0
2	Q	1	Total 6	C 3	O 3	0	0
2	Q	1	Total 6	C 3	O 3	0	0
2	R	1	Total 6	C 3	O 3	0	0
2	R	1	Total 6	C 3	O 3	0	0
2	R	1	Total 6	C 3	O 3	0	0
2	S	1	Total 6	C 3	O 3	0	0
2	S	1	Total 6	C 3	O 3	0	0
2	S	1	Total 6	C 3	O 3	0	0
2	T	1	Total 6	C 3	O 3	0	0
2	T	1	Total 6	C 3	O 3	0	0
2	T	1	Total 6	C 3	O 3	0	0
2	U	1	Total 6	C 3	O 3	0	0
2	U	1	Total 6	C 3	O 3	0	0
2	U	1	Total 6	C 3	O 3	0	0
2	V	1	Total 6	C 3	O 3	0	0
2	V	1	Total 6	C 3	O 3	0	0
2	V	1	Total 6	C 3	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	98	Total	O	0	0
			98	98		
3	C	100	Total	O	0	0
			100	100		
3	D	96	Total	O	0	0
			96	96		
3	E	93	Total	O	0	0
			93	93		
3	F	91	Total	O	0	0
			91	91		
3	G	91	Total	O	0	0
			91	91		
3	H	75	Total	O	0	0
			75	75		
3	I	91	Total	O	0	0
			91	91		
3	J	91	Total	O	0	0
			91	91		
3	K	83	Total	O	0	0
			83	83		
3	L	86	Total	O	0	0
			86	86		
3	M	97	Total	O	0	0
			97	97		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	96	Total 96	O 96	0	0
3	O	89	Total 89	O 89	0	0
3	P	97	Total 97	O 97	0	0
3	Q	97	Total 97	O 97	0	0
3	R	103	Total 103	O 103	0	0
3	S	84	Total 84	O 84	0	0
3	T	87	Total 87	O 87	0	0
3	U	101	Total 101	O 101	0	0
3	V	107	Total 107	O 107	0	0
3	X	79	Total 79	O 79	0	0
3	Y	80	Total 80	O 80	0	0

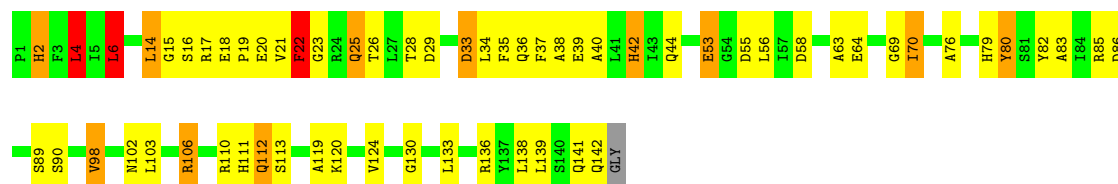
3 Residue-property plots

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

Note EDS was not executed.

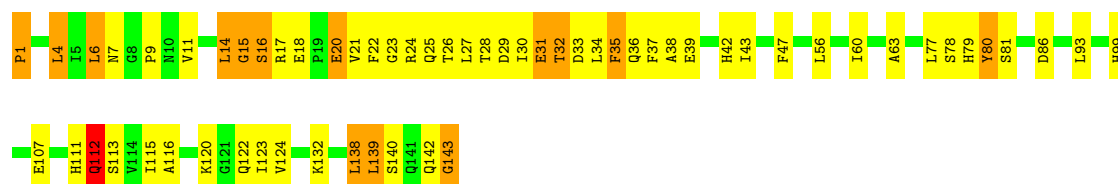
• Molecule 1: DEHYDROQUINASE

Chain A: 



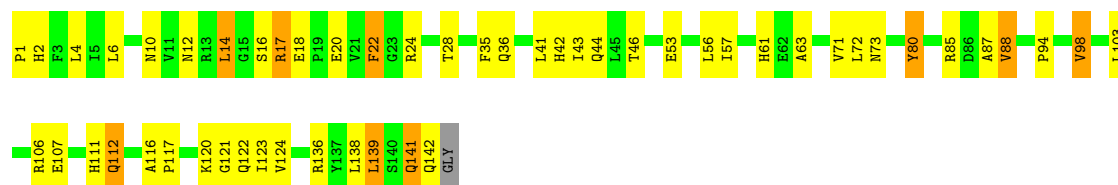
• Molecule 1: DEHYDROQUINASE

Chain B: 



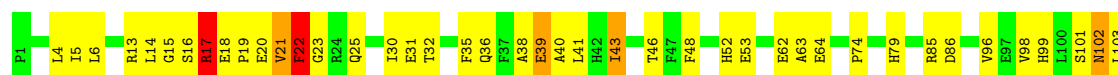
• Molecule 1: DEHYDROQUINASE

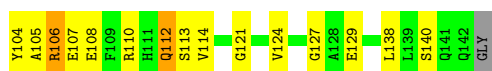
Chain C: 



• Molecule 1: DEHYDROQUINASE

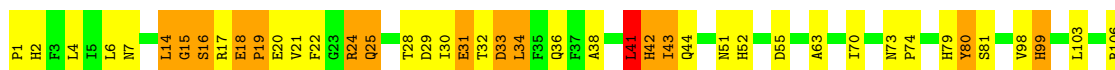
Chain D: 





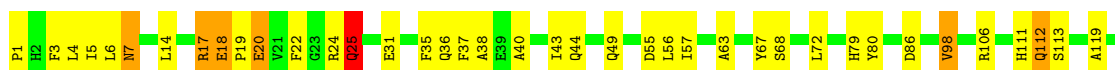
• Molecule 1: DEHYDROQUINASE

Chain E: 59% 29% 10% ..



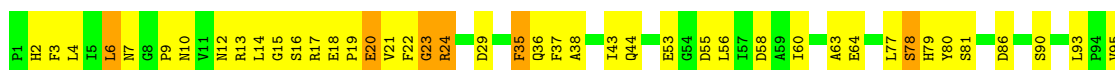
• Molecule 1: DEHYDROQUINASE

Chain F: 68% 26% 5% ..



• Molecule 1: DEHYDROQUINASE

Chain G: 55% 38% 5% ..



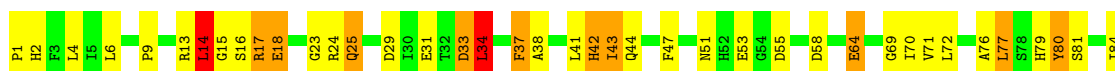
• Molecule 1: DEHYDROQUINASE

Chain H: 54% 32% 11% ..



• Molecule 1: DEHYDROQUINASE

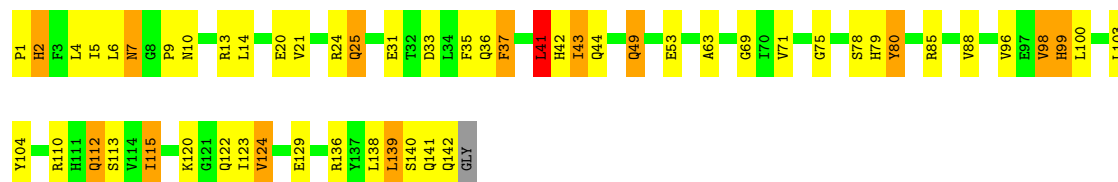
Chain I: 55% 34% 8% ..





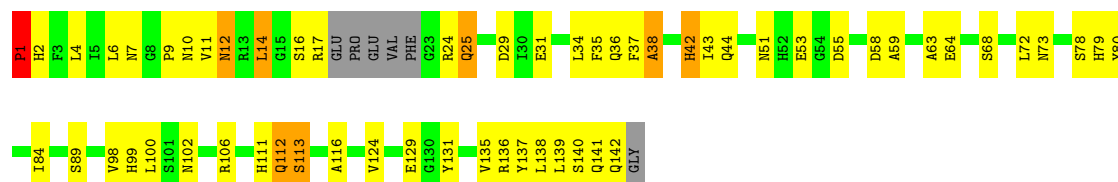
• Molecule 1: DEHYDROQUINASE

Chain J: 61% 29% 9% ..



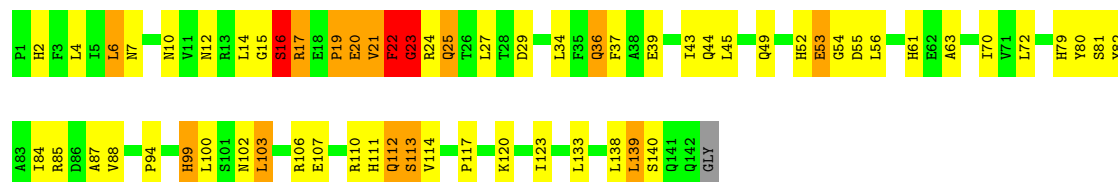
• Molecule 1: DEHYDROQUINASE

Chain K: 55% 36% 5% ..



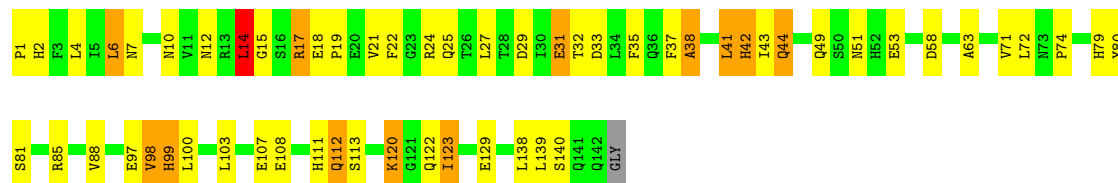
• Molecule 1: DEHYDROQUINASE

Chain L: 55% 33% 9% ..



• Molecule 1: DEHYDROQUINASE

Chain M: 59% 31% 8% ..



• Molecule 1: DEHYDROQUINASE

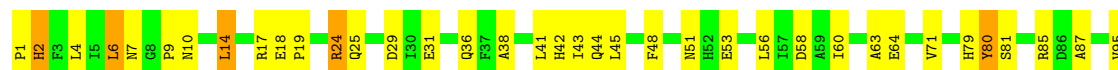
Chain N: 57% 31% 7% ..





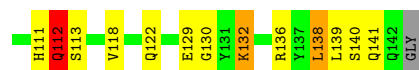
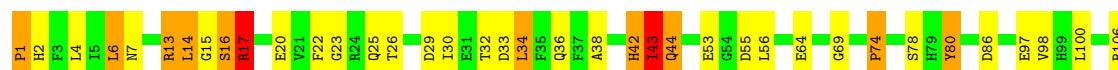
• Molecule 1: DEHYDROQUINASE

Chain O: 59% 35% ..



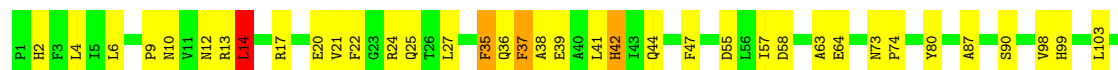
• Molecule 1: DEHYDROQUINASE

Chain P: 64% 25% 8% ..



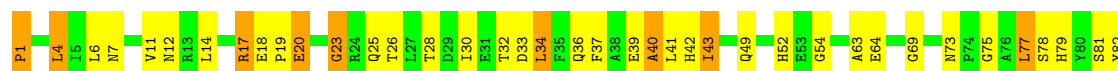
• Molecule 1: DEHYDROQUINASE

Chain Q: 64% 30% ..



• Molecule 1: DEHYDROQUINASE

Chain R: 59% 31% 8% ..



• Molecule 1: DEHYDROQUINASE

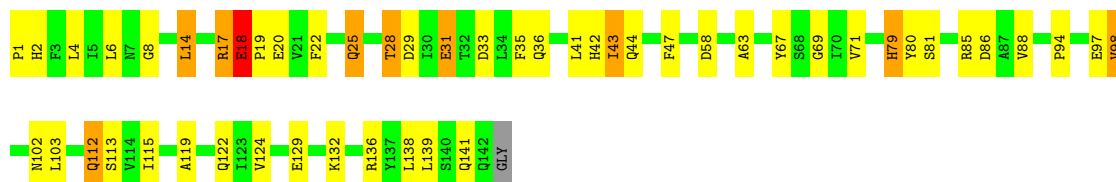
Chain S: 60% 31% 7% ..





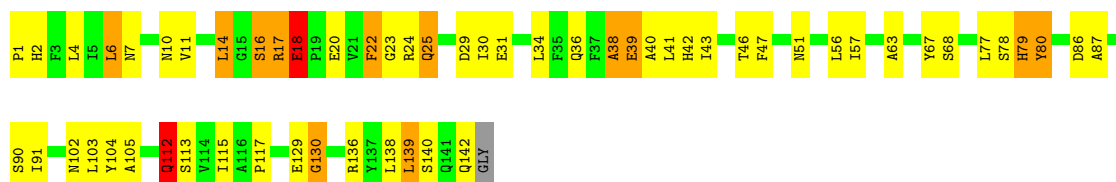
• Molecule 1: DEHYDROQUINASE

Chain T: 64% 29% 6% ..



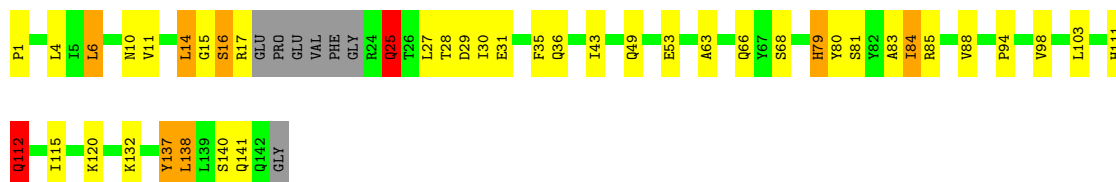
• Molecule 1: DEHYDROQUINASE

Chain U: 59% 31% 8% ..



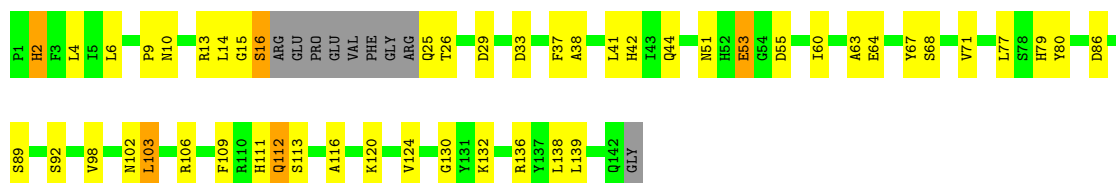
• Molecule 1: DEHYDROQUINASE

Chain V: 66% 23% 5% • 5%



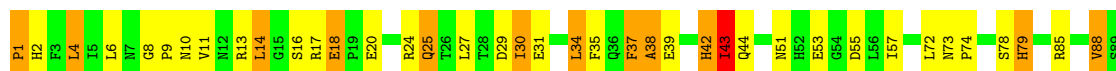
• Molecule 1: DEHYDROQUINASE

Chain X: 59% 31% • 6%



• Molecule 1: DEHYDROQUINASE

Chain Y: 57% 31% 10% ..





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.21Å 195.61Å 97.36Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	21.84 – 2.10	Depositor
% Data completeness (in resolution range)	86.0 (21.84-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
 GOL

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	1.22	1/1117 (0.1%)	2.32	57/1519 (3.8%)
1	B	2.51	5/1128 (0.4%)	2.11	40/1529 (2.6%)
1	C	1.25	1/1116 (0.1%)	2.12	51/1518 (3.4%)
1	D	1.23	0/1122	2.24	52/1526 (3.4%)
1	E	1.65	2/1143 (0.2%)	2.67	58/1554 (3.7%)
1	F	1.19	0/1146	2.12	41/1558 (2.6%)
1	G	1.22	3/1135 (0.3%)	2.12	44/1543 (2.9%)
1	H	1.66	2/1121 (0.2%)	2.58	66/1525 (4.3%)
1	I	1.29	3/1113 (0.3%)	2.26	49/1514 (3.2%)
1	J	1.16	1/1116 (0.1%)	2.09	45/1518 (3.0%)
1	K	1.30	4/1071 (0.4%)	2.27	58/1454 (4.0%)
1	L	1.30	1/1112 (0.1%)	2.32	58/1513 (3.8%)
1	M	1.24	3/1126 (0.3%)	2.17	49/1530 (3.2%)
1	N	1.28	2/1048 (0.2%)	2.18	42/1424 (2.9%)
1	O	1.19	0/1119	2.25	56/1521 (3.7%)
1	P	1.23	0/1123	2.20	39/1527 (2.6%)
1	Q	1.25	3/1133 (0.3%)	2.22	47/1539 (3.1%)
1	R	1.22	0/1122	2.25	56/1526 (3.7%)
1	S	1.25	2/1132 (0.2%)	2.18	42/1538 (2.7%)
1	T	1.18	1/1133 (0.1%)	2.14	45/1540 (2.9%)
1	U	1.32	3/1116 (0.3%)	2.24	42/1518 (2.8%)
1	V	1.18	0/1077	2.03	30/1462 (2.1%)
1	X	1.25	1/1054 (0.1%)	2.22	49/1432 (3.4%)
1	Y	1.24	4/1120 (0.4%)	2.25	55/1523 (3.6%)
All	All	1.35	42/26743 (0.2%)	2.24	1171/36351 (3.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	H	0	1
1	I	0	1
1	K	0	1
1	R	0	1
1	X	0	1
All	All	0	6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLY	C-OXT	72.90	2.69	1.23
1	H	141	GLN	C-N	38.32	1.86	1.33
1	E	141	GLN	C-N	-35.40	0.83	1.33
1	E	119	ALA	C-N	7.97	1.45	1.34
1	K	98	VAL	C-O	7.79	1.31	1.24
1	K	124	VAL	C-O	-7.50	1.16	1.24
1	K	111	HIS	CD2-NE2	-7.32	1.29	1.37
1	U	79	HIS	CD2-NE2	-6.55	1.30	1.37
1	Q	136	ARG	C-N	6.19	1.42	1.33
1	A	98	VAL	N-CA	-6.09	1.39	1.46
1	Y	136	ARG	NE-CZ	6.09	1.39	1.33
1	M	71	VAL	CA-CB	-6.05	1.47	1.54
1	M	99	HIS	CE1-NE2	6.05	1.38	1.32
1	C	121	GLY	N-CA	5.94	1.53	1.45
1	M	10	ASN	CG-OD1	5.86	1.34	1.23
1	I	95	VAL	C-N	-5.84	1.26	1.33
1	U	57	ILE	C-N	-5.82	1.26	1.33
1	I	116	ALA	CA-C	-5.81	1.45	1.52
1	G	60	ILE	C-O	-5.73	1.17	1.24
1	B	124	VAL	C-O	-5.58	1.18	1.24
1	B	122	GLN	CA-CB	5.54	1.63	1.53
1	N	7	ASN	C-O	-5.48	1.17	1.24
1	K	116	ALA	CA-C	-5.47	1.46	1.52
1	U	130	GLY	C-N	-5.42	1.27	1.33
1	S	120	LYS	CA-CB	5.41	1.61	1.53
1	Y	73	ASN	N-CA	-5.40	1.41	1.46
1	G	78	SER	CA-C	5.35	1.59	1.52
1	J	113	SER	N-CA	-5.35	1.39	1.46
1	Y	79	HIS	CE1-NE2	-5.34	1.27	1.32
1	I	104	TYR	N-CA	-5.26	1.39	1.46
1	Q	24	ARG	CD-NE	-5.20	1.39	1.46
1	S	71	VAL	CA-CB	-5.19	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	119	ALA	C-N	-5.18	1.26	1.33
1	L	61	HIS	CD2-NE2	-5.16	1.32	1.37
1	X	124	VAL	C-O	-5.15	1.19	1.24
1	G	10	ASN	C-N	-5.13	1.27	1.33
1	B	93	LEU	C-O	5.12	1.30	1.23
1	B	7	ASN	N-CA	-5.12	1.39	1.46
1	N	97	GLU	CA-CB	5.09	1.60	1.53
1	H	103	LEU	C-N	-5.07	1.27	1.33
1	T	85	ARG	CD-NE	-5.05	1.39	1.46
1	Y	9	PRO	N-CA	-5.01	1.41	1.47

All (1171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	141	GLN	O-C-N	-54.13	36.39	123.00
1	H	141	GLN	CA-C-N	-29.14	57.92	116.20
1	H	141	GLN	O-C-N	-27.52	78.96	123.00
1	A	33	ASP	CA-CB-CG	26.13	138.73	112.60
1	O	36	GLN	CB-CG-CD	20.32	147.14	112.60
1	Q	42	HIS	CA-CB-CG	-18.41	95.39	113.80
1	Q	24	ARG	CD-NE-CZ	17.84	149.38	124.40
1	H	41	LEU	CA-C-N	16.86	145.96	122.19
1	H	41	LEU	C-N-CA	16.86	145.96	122.19
1	I	33	ASP	CA-CB-CG	16.12	128.72	112.60
1	D	31	GLU	CA-CB-CG	15.93	145.95	114.10
1	A	42	HIS	CA-CB-CG	-15.83	97.97	113.80
1	S	141	GLN	OE1-CD-NE2	15.46	138.06	122.60
1	I	43	ILE	CA-C-O	15.16	136.31	120.39
1	R	17	ARG	CD-NE-CZ	15.01	145.42	124.40
1	L	110	ARG	CD-NE-CZ	13.93	143.90	124.40
1	P	33	ASP	CA-CB-CG	13.40	126.00	112.60
1	H	41	LEU	CA-C-O	13.32	139.56	120.51
1	U	112	GLN	CB-CG-CD	13.01	134.71	112.60
1	H	112	GLN	CB-CG-CD	12.68	134.16	112.60
1	M	29	ASP	CA-CB-CG	12.64	125.24	112.60
1	C	112	GLN	CB-CG-CD	12.32	133.54	112.60
1	M	33	ASP	CA-CB-CG	12.11	124.71	112.60
1	K	42	HIS	CA-CB-CG	12.09	125.89	113.80
1	E	41	LEU	CA-C-O	12.04	134.15	119.95
1	G	35	PHE	CA-CB-CG	-11.93	101.87	113.80
1	B	37	PHE	CA-CB-CG	11.74	125.54	113.80
1	V	112	GLN	CB-CG-CD	11.73	132.55	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	24	ARG	CD-NE-CZ	11.71	140.79	124.40
1	S	112	GLN	CB-CG-CD	11.62	132.35	112.60
1	R	112	GLN	CB-CG-CD	11.24	131.72	112.60
1	M	17	ARG	CG-CD-NE	11.09	136.39	112.00
1	H	43	ILE	CA-C-O	11.01	135.39	121.40
1	H	41	LEU	O-C-N	-10.97	108.00	122.59
1	E	141	GLN	CA-C-N	-10.86	94.48	116.20
1	Q	112	GLN	CB-CG-CD	10.86	131.06	112.60
1	G	29	ASP	CA-CB-CG	10.82	123.42	112.60
1	E	18	GLU	N-CA-C	10.77	125.01	109.71
1	L	17	ARG	CD-NE-CZ	10.49	139.09	124.40
1	R	41	LEU	CA-C-N	10.44	137.18	122.36
1	R	41	LEU	C-N-CA	10.44	137.18	122.36
1	I	112	GLN	CB-CG-CD	10.43	130.33	112.60
1	E	29	ASP	CA-CB-CG	10.39	122.99	112.60
1	I	37	PHE	CA-CB-CG	10.36	124.16	113.80
1	P	112	GLN	CB-CG-CD	10.20	129.93	112.60
1	P	43	ILE	CA-C-O	10.19	133.10	121.28
1	X	37	PHE	CA-CB-CG	10.14	123.94	113.80
1	F	36	GLN	OE1-CD-NE2	-10.13	112.47	122.60
1	Y	37	PHE	CA-CB-CG	10.13	123.93	113.80
1	Q	17	ARG	CD-NE-CZ	10.05	138.48	124.40
1	E	112	GLN	CB-CG-CD	10.02	129.63	112.60
1	K	29	ASP	CA-CB-CG	10.02	122.62	112.60
1	H	17	ARG	CD-NE-CZ	10.00	138.40	124.40
1	D	85	ARG	NE-CZ-NH2	9.95	128.16	119.20
1	D	15	GLY	N-CA-C	9.86	124.13	113.58
1	Q	112	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	G	118	VAL	O-C-N	-9.74	113.30	122.16
1	O	29	ASP	CA-CB-CG	9.74	122.34	112.60
1	Y	55	ASP	CA-CB-CG	9.73	122.33	112.60
1	S	42	HIS	CA-CB-CG	-9.62	104.18	113.80
1	M	112	GLN	CB-CG-CD	9.62	128.95	112.60
1	O	112	GLN	CB-CG-CD	9.60	128.92	112.60
1	J	112	GLN	CB-CG-CD	9.57	128.87	112.60
1	T	122	GLN	OE1-CD-NE2	-9.51	113.09	122.60
1	P	138	LEU	CA-C-N	9.50	133.19	120.65
1	P	138	LEU	C-N-CA	9.50	133.19	120.65
1	H	40	ALA	N-CA-CB	9.43	126.12	111.22
1	H	37	PHE	CA-CB-CG	9.38	123.19	113.80
1	C	112	GLN	OE1-CD-NE2	-9.33	113.27	122.60
1	X	112	GLN	OE1-CD-NE2	-9.30	113.30	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	98	VAL	O-C-N	-9.29	113.16	123.10
1	R	39	GLU	CA-C-O	-9.29	109.79	120.20
1	N	114	VAL	CA-CB-CG2	9.27	126.15	110.40
1	G	22	PHE	CA-CB-CG	9.25	123.05	113.80
1	Y	42	HIS	CA-CB-CG	-9.21	104.59	113.80
1	I	24	ARG	N-CA-C	9.21	124.65	113.23
1	K	24	ARG	CA-C-O	9.16	130.84	119.11
1	M	112	GLN	OE1-CD-NE2	-9.14	113.46	122.60
1	E	42	HIS	CA-CB-CG	-9.13	104.67	113.80
1	T	112	GLN	CB-CG-CD	9.08	128.03	112.60
1	X	55	ASP	CA-CB-CG	9.06	121.66	112.60
1	Y	39	GLU	CA-C-O	9.05	130.02	120.70
1	Q	25	GLN	OE1-CD-NE2	9.03	131.63	122.60
1	A	112	GLN	CB-CG-CD	9.02	127.94	112.60
1	B	23	GLY	CA-C-N	8.99	132.70	120.38
1	B	23	GLY	C-N-CA	8.99	132.70	120.38
1	E	55	ASP	CA-CB-CG	8.87	121.47	112.60
1	U	129	GLU	CA-C-N	8.86	129.95	120.03
1	U	129	GLU	C-N-CA	8.86	129.95	120.03
1	B	112	GLN	CB-CG-CD	8.86	127.66	112.60
1	R	140	SER	CA-C-O	-8.86	110.28	120.20
1	G	9	PRO	CA-C-O	8.83	131.41	121.34
1	S	17	ARG	CA-CB-CG	8.83	131.76	114.10
1	L	34	LEU	N-CA-CB	8.72	123.06	110.16
1	X	29	ASP	CA-CB-CG	8.71	121.31	112.60
1	N	112	GLN	OE1-CD-NE2	-8.71	113.89	122.60
1	K	98	VAL	O-C-N	-8.70	113.79	123.18
1	B	139	LEU	N-CA-CB	8.68	122.60	110.01
1	S	107	GLU	CA-C-N	8.63	131.85	120.28
1	S	107	GLU	C-N-CA	8.63	131.85	120.28
1	D	17	ARG	CD-NE-CZ	8.63	136.48	124.40
1	M	25	GLN	OE1-CD-NE2	8.60	131.20	122.60
1	E	106	ARG	NH1-CZ-NH2	-8.57	108.15	119.30
1	S	73	ASN	CA-C-O	8.57	129.21	120.38
1	S	85	ARG	CD-NE-CZ	8.57	136.39	124.40
1	E	106	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	N	85	ARG	NH1-CZ-NH2	-8.50	108.25	119.30
1	P	69	GLY	CA-C-O	-8.49	113.34	121.49
1	R	112	GLN	OE1-CD-NE2	-8.47	114.13	122.60
1	Y	100	LEU	CA-C-O	-8.47	111.49	120.55
1	X	26	THR	CA-CB-CG2	8.38	124.75	110.50
1	A	112	GLN	OE1-CD-NE2	-8.35	114.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	106	ARG	CD-NE-CZ	8.33	136.06	124.40
1	U	112	GLN	OE1-CD-NE2	-8.30	114.30	122.60
1	A	29	ASP	CA-CB-CG	8.28	120.88	112.60
1	F	31	GLU	CB-CG-CD	8.25	126.63	112.60
1	P	86	ASP	CA-CB-CG	8.25	120.85	112.60
1	A	80	TYR	CA-CB-CG	8.25	128.75	113.90
1	G	98	VAL	O-C-N	-8.24	114.30	123.20
1	L	36	GLN	CG-CD-NE2	8.24	128.76	116.40
1	I	55	ASP	CA-CB-CG	8.24	120.84	112.60
1	I	130	GLY	O-C-N	-8.23	114.29	122.19
1	I	80	TYR	CA-CB-CG	8.22	128.70	113.90
1	T	17	ARG	CD-NE-CZ	8.21	135.90	124.40
1	L	63	ALA	CA-C-N	8.18	131.59	120.38
1	L	63	ALA	C-N-CA	8.18	131.59	120.38
1	Y	31	GLU	CA-CB-CG	8.16	130.41	114.10
1	H	79	HIS	CA-CB-CG	-8.14	105.66	113.80
1	R	41	LEU	CA-C-O	8.13	132.14	120.51
1	F	7	ASN	OD1-CG-ND2	-8.10	114.50	122.60
1	L	22	PHE	CA-C-O	8.10	132.10	120.51
1	I	23	GLY	CA-C-O	-8.09	115.73	122.29
1	S	139	LEU	CB-CA-C	-8.08	98.19	110.88
1	C	80	TYR	CA-CB-CG	8.05	128.39	113.90
1	X	51	ASN	CA-C-N	8.04	133.16	122.30
1	X	51	ASN	C-N-CA	8.04	133.16	122.30
1	H	112	GLN	OE1-CD-NE2	-8.04	114.56	122.60
1	T	33	ASP	CA-CB-CG	-8.03	104.57	112.60
1	I	42	HIS	CA-CB-CG	-7.98	105.82	113.80
1	V	49	GLN	OE1-CD-NE2	-7.98	114.62	122.60
1	I	109	PHE	O-C-N	-7.92	112.09	122.39
1	K	31	GLU	CA-CB-CG	7.91	129.92	114.10
1	K	73	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	H	42	HIS	CA-C-O	7.88	130.66	121.28
1	S	30	ILE	N-CA-CB	-7.86	101.35	110.55
1	X	63	ALA	CA-C-N	7.84	131.13	120.38
1	X	63	ALA	C-N-CA	7.84	131.13	120.38
1	A	35	PHE	CA-C-O	-7.84	112.77	121.00
1	A	33	ASP	N-CA-CB	7.83	121.63	110.12
1	O	36	GLN	CG-CD-NE2	7.82	128.13	116.40
1	Y	118	VAL	O-C-N	7.81	129.27	122.16
1	H	12	ASN	OD1-CG-ND2	-7.77	114.83	122.60
1	L	87	ALA	N-CA-C	-7.77	102.75	111.14
1	I	138	LEU	CA-C-N	7.74	131.28	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	138	LEU	C-N-CA	7.74	131.28	120.29
1	S	35	PHE	CA-CB-CG	-7.73	106.07	113.80
1	Y	39	GLU	CA-C-N	7.71	135.33	120.99
1	Y	39	GLU	C-N-CA	7.71	135.33	120.99
1	D	22	PHE	CA-CB-CG	7.69	121.49	113.80
1	O	2	HIS	CA-CB-CG	7.65	121.45	113.80
1	M	12	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	N	39	GLU	CA-C-O	-7.63	112.74	120.90
1	Y	79	HIS	CA-CB-CG	-7.62	106.18	113.80
1	K	59	ALA	O-C-N	-7.62	114.05	122.12
1	N	85	ARG	NE-CZ-NH2	7.61	126.05	119.20
1	H	43	ILE	O-C-N	-7.60	115.08	122.98
1	Y	97	GLU	O-C-N	-7.59	114.35	123.16
1	M	63	ALA	CA-C-N	7.58	130.76	120.38
1	M	63	ALA	C-N-CA	7.58	130.76	120.38
1	F	98	VAL	O-C-N	-7.56	115.01	123.10
1	L	22	PHE	CA-C-N	7.56	136.23	121.41
1	L	22	PHE	C-N-CA	7.56	136.23	121.41
1	O	115	ILE	CA-C-O	7.56	127.86	119.92
1	G	136	ARG	O-C-N	-7.56	114.11	122.12
1	J	37	PHE	CA-C-O	7.53	129.35	120.92
1	V	137	TYR	O-C-N	-7.53	114.32	122.07
1	I	112	GLN	OE1-CD-NE2	-7.52	115.08	122.60
1	A	69	GLY	O-C-N	-7.51	115.10	123.66
1	B	80	TYR	CA-CB-CG	7.51	127.42	113.90
1	K	1	PRO	CA-N-CD	-7.51	101.49	112.00
1	K	11	VAL	CA-C-O	7.50	128.80	120.85
1	K	35	PHE	N-CA-C	-7.49	103.05	111.07
1	T	88	VAL	O-C-N	-7.49	114.60	121.87
1	A	103	LEU	O-C-N	-7.49	114.18	122.12
1	F	35	PHE	CA-CB-CG	-7.49	106.31	113.80
1	T	42	HIS	CA-CB-CG	-7.46	106.34	113.80
1	D	108	GLU	O-C-N	-7.45	114.23	122.12
1	G	15	GLY	N-CA-C	7.43	123.32	114.48
1	K	112	GLN	CB-CG-CD	7.43	125.23	112.60
1	L	22	PHE	O-C-N	-7.43	112.71	122.59
1	Q	98	VAL	CA-C-O	7.43	128.93	120.76
1	J	112	GLN	OE1-CD-NE2	-7.41	115.19	122.60
1	H	72	LEU	O-C-N	7.38	131.83	123.27
1	F	80	TYR	CA-CB-CG	7.38	127.19	113.90
1	K	80	TYR	CA-CB-CG	7.38	127.18	113.90
1	J	13	ARG	NE-CZ-NH1	-7.37	114.13	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	79	HIS	CA-CB-CG	-7.37	106.43	113.80
1	E	52	HIS	CA-CB-CG	-7.36	106.44	113.80
1	R	12	ASN	OD1-CG-ND2	-7.36	115.24	122.60
1	X	112	GLN	CB-CG-CD	7.36	125.11	112.60
1	I	85	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	R	30	ILE	CB-CA-C	-7.35	102.57	111.97
1	I	95	VAL	CA-C-N	7.33	132.86	123.10
1	I	95	VAL	C-N-CA	7.33	132.86	123.10
1	D	129	GLU	O-C-N	-7.32	113.86	122.20
1	K	55	ASP	CA-CB-CG	7.31	119.91	112.60
1	V	84	ILE	O-C-N	-7.30	114.31	121.83
1	H	42	HIS	CB-CA-C	-7.30	101.37	111.73
1	M	79	HIS	CB-CG-CD2	-7.29	121.73	131.20
1	O	124	VAL	CA-C-O	-7.28	112.52	120.67
1	N	112	GLN	CG-CD-NE2	7.27	127.31	116.40
1	Q	137	TYR	CA-C-O	7.26	128.25	120.55
1	O	36	GLN	CA-C-N	7.25	130.31	120.38
1	O	36	GLN	C-N-CA	7.25	130.31	120.38
1	D	35	PHE	CA-C-N	7.25	130.31	120.38
1	D	35	PHE	C-N-CA	7.25	130.31	120.38
1	O	60	ILE	N-CA-C	-7.25	103.72	110.53
1	N	112	GLN	CB-CG-CD	7.24	124.91	112.60
1	V	88	VAL	O-C-N	-7.24	114.85	121.87
1	U	16	SER	CA-C-N	7.23	134.17	122.53
1	U	16	SER	C-N-CA	7.23	134.17	122.53
1	I	43	ILE	O-C-N	-7.21	115.47	123.26
1	E	16[A]	SER	CA-C-N	7.21	135.30	121.54
1	E	16[A]	SER	C-N-CA	7.21	135.30	121.54
1	E	16[B]	SER	CA-C-N	7.21	135.30	121.54
1	E	16[B]	SER	C-N-CA	7.21	135.30	121.54
1	F	35	PHE	CA-C-N	7.20	129.93	120.28
1	F	35	PHE	C-N-CA	7.20	129.93	120.28
1	G	99	HIS	CA-CB-CG	-7.20	106.60	113.80
1	D	53	GLU	CA-C-N	7.19	129.13	120.14
1	D	53	GLU	C-N-CA	7.19	129.13	120.14
1	U	23	GLY	N-CA-C	-7.18	103.31	112.65
1	D	15	GLY	O-C-N	-7.18	116.97	122.71
1	B	42	HIS	CA-CB-CG	-7.17	106.63	113.80
1	E	19	PRO	CA-C-N	7.17	131.20	120.31
1	E	19	PRO	C-N-CA	7.17	131.20	120.31
1	T	67	TYR	CA-C-O	-7.16	113.27	121.58
1	N	110	ARG	CD-NE-CZ	7.16	134.42	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	39	GLU	CA-C-O	-7.16	112.90	120.63
1	Y	24	ARG	CA-C-O	7.15	128.00	120.42
1	R	110	ARG	CD-NE-CZ	7.14	134.40	124.40
1	H	33	ASP	CA-CB-CG	7.14	119.74	112.60
1	U	34	LEU	CA-C-N	7.12	130.16	120.54
1	U	34	LEU	C-N-CA	7.12	130.16	120.54
1	D	124	VAL	O-C-N	-7.12	115.48	123.10
1	R	104	TYR	CA-C-O	7.12	128.10	119.49
1	F	17	ARG	CD-NE-CZ	7.11	134.36	124.40
1	C	10	ASN	OD1-CG-ND2	7.10	129.70	122.60
1	S	106	ARG	CD-NE-CZ	7.10	134.34	124.40
1	T	102	ASN	OD1-CG-ND2	7.10	129.70	122.60
1	D	63	ALA	CA-C-N	7.10	130.74	120.38
1	D	63	ALA	C-N-CA	7.10	130.74	120.38
1	B	112	GLN	OE1-CD-NE2	-7.08	115.52	122.60
1	N	82	TYR	CB-CG-CD2	7.08	131.42	120.80
1	O	71	VAL	N-CA-CB	7.07	120.58	111.67
1	G	132	LYS	CA-C-O	7.07	127.98	120.70
1	E	80	TYR	CA-CB-CG	7.06	126.60	113.90
1	X	86	ASP	O-C-N	-7.06	113.96	122.22
1	Q	37	PHE	CA-CB-CG	7.05	120.85	113.80
1	K	24	ARG	CA-C-N	7.04	133.78	120.97
1	K	24	ARG	C-N-CA	7.04	133.78	120.97
1	V	25	GLN	CB-CG-CD	-7.02	100.66	112.60
1	O	87	ALA	CA-C-N	7.02	130.07	120.46
1	O	87	ALA	C-N-CA	7.02	130.07	120.46
1	L	103	LEU	O-C-N	-7.00	114.21	122.20
1	L	106	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	A	63	ALA	CA-C-N	7.00	130.60	120.38
1	A	63	ALA	C-N-CA	7.00	130.60	120.38
1	E	112	GLN	OE1-CD-NE2	-7.00	115.60	122.60
1	T	141	GLN	OE1-CD-NE2	7.00	129.59	122.60
1	R	49	GLN	CA-C-O	-6.99	113.15	120.70
1	T	85	ARG	NE-CZ-NH1	-6.97	114.53	121.50
1	T	41	LEU	CA-C-O	6.97	128.38	119.95
1	E	33	ASP	CB-CA-C	-6.96	99.25	110.79
1	Y	88	VAL	CA-C-O	-6.95	113.72	120.95
1	L	53	GLU	CA-C-N	6.94	127.69	119.98
1	L	53	GLU	C-N-CA	6.94	127.69	119.98
1	H	103	LEU	CA-C-N	6.94	131.71	120.60
1	H	103	LEU	C-N-CA	6.94	131.71	120.60
1	C	41	LEU	O-C-N	6.94	130.63	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	68	SER	O-C-N	-6.92	113.86	122.24
1	Q	14	LEU	CA-C-N	6.92	133.46	121.07
1	Q	14	LEU	C-N-CA	6.92	133.46	121.07
1	O	58	ASP	CA-C-N	6.92	129.55	120.28
1	O	58	ASP	C-N-CA	6.92	129.55	120.28
1	X	136	ARG	NE-CZ-NH2	6.91	125.42	119.20
1	S	119	ALA	CA-C-O	6.90	130.17	121.82
1	N	100	LEU	O-C-N	6.88	129.52	122.09
1	B	38	ALA	N-CA-C	6.88	118.57	111.14
1	F	136	ARG	O-C-N	-6.88	114.83	122.12
1	D	99	HIS	CA-CB-CG	-6.86	106.94	113.80
1	F	3	PHE	CA-C-N	6.86	132.19	122.72
1	F	3	PHE	C-N-CA	6.86	132.19	122.72
1	O	36	GLN	OE1-CD-NE2	-6.86	115.74	122.60
1	E	79	HIS	CA-C-O	-6.85	110.99	119.28
1	L	36	GLN	OE1-CD-NE2	-6.85	115.75	122.60
1	R	30	ILE	N-CA-CB	6.85	118.56	110.55
1	T	69	GLY	CA-C-O	-6.84	114.92	121.49
1	S	39	GLU	CA-C-O	-6.83	113.31	120.55
1	D	121	GLY	CA-C-O	-6.83	114.79	121.75
1	G	37	PHE	CA-CB-CG	6.82	120.62	113.80
1	P	26	THR	CA-C-O	-6.82	113.87	121.51
1	D	129	GLU	CA-C-N	6.82	128.66	120.14
1	D	129	GLU	C-N-CA	6.82	128.66	120.14
1	V	1	PRO	CA-N-CD	-6.82	102.46	112.00
1	Y	85	ARG	CA-C-N	6.80	130.65	120.31
1	Y	85	ARG	C-N-CA	6.80	130.65	120.31
1	E	119	ALA	CA-C-N	-6.79	109.98	120.31
1	E	119	ALA	C-N-CA	-6.79	109.98	120.31
1	B	138	LEU	N-CA-C	-6.79	103.81	111.14
1	T	85	ARG	CD-NE-CZ	6.78	133.90	124.40
1	S	13	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	T	79	HIS	N-CA-C	6.78	121.41	113.20
1	O	131	TYR	O-C-N	-6.78	114.93	122.12
1	C	136	ARG	NE-CZ-NH2	6.77	125.30	119.20
1	Q	24	ARG	CA-C-O	-6.75	113.23	121.06
1	R	37	PHE	CA-CB-CG	6.73	120.53	113.80
1	R	75	GLY	O-C-N	-6.72	115.22	122.95
1	H	39	GLU	CA-C-O	-6.72	110.31	119.05
1	S	33	ASP	CA-CB-CG	-6.72	105.88	112.60
1	R	28	THR	N-CA-CB	6.72	120.10	110.16
1	C	61	HIS	CA-C-N	6.71	131.92	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	HIS	C-N-CA	6.71	131.92	120.72
1	J	42	HIS	CA-C-N	6.71	132.22	122.69
1	J	42	HIS	C-N-CA	6.71	132.22	122.69
1	Q	80	TYR	CA-CB-CG	6.71	125.98	113.90
1	R	40	ALA	CA-C-O	-6.71	113.16	121.88
1	D	86	ASP	CA-C-N	6.70	129.15	120.44
1	D	86	ASP	C-N-CA	6.70	129.15	120.44
1	V	16	SER	N-CA-C	6.69	125.06	110.80
1	Y	24	ARG	CA-C-N	6.69	132.86	120.95
1	Y	24	ARG	C-N-CA	6.69	132.86	120.95
1	Q	107	GLU	CA-C-N	6.68	129.90	120.28
1	Q	107	GLU	C-N-CA	6.68	129.90	120.28
1	Y	112	GLN	CB-CG-CD	6.68	123.95	112.60
1	P	17	ARG	CD-NE-CZ	6.66	133.73	124.40
1	H	42	HIS	CA-CB-CG	6.66	120.46	113.80
1	J	112	GLN	CG-CD-NE2	6.66	126.39	116.40
1	I	58	ASP	CA-CB-CG	6.65	119.25	112.60
1	Q	55	ASP	CA-CB-CG	6.65	119.25	112.60
1	F	40	ALA	CA-C-N	6.65	132.15	121.98
1	F	40	ALA	C-N-CA	6.65	132.15	121.98
1	K	112	GLN	OE1-CD-NE2	-6.64	115.96	122.60
1	E	36	GLN	CA-C-O	6.64	127.54	120.70
1	E	99	HIS	CA-CB-CG	-6.63	107.17	113.80
1	L	17	ARG	NE-CZ-NH2	6.63	125.16	119.20
1	X	9	PRO	N-CA-CB	6.62	109.20	103.31
1	G	58	ASP	CA-CB-CG	6.62	119.22	112.60
1	T	28	THR	N-CA-CB	6.62	119.85	110.12
1	H	34	LEU	N-CA-CB	6.62	120.54	110.28
1	O	7	ASN	CA-CB-CG	6.62	119.22	112.60
1	Q	99	HIS	CA-CB-CG	-6.61	107.19	113.80
1	I	17	ARG	CA-C-N	6.60	137.91	121.80
1	I	17	ARG	C-N-CA	6.60	137.91	121.80
1	G	36	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	C	98	VAL	O-C-N	-6.59	116.06	123.18
1	H	34	LEU	O-C-N	-6.58	114.17	122.27
1	P	36	GLN	CA-C-O	6.58	127.73	120.82
1	V	83	ALA	CA-C-O	-6.58	113.58	120.55
1	A	35	PHE	O-C-N	6.58	128.87	122.03
1	D	15	GLY	CA-C-N	6.58	129.75	120.28
1	D	15	GLY	C-N-CA	6.58	129.75	120.28
1	V	43	ILE	O-C-N	-6.58	115.93	122.97
1	Q	57	ILE	O-C-N	-6.57	115.47	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	139	LEU	CA-C-O	-6.56	111.55	119.49
1	O	48	PHE	CA-C-O	-6.56	112.47	120.54
1	O	25	GLN	N-CA-C	6.56	119.19	110.53
1	U	25	GLN	CB-CG-CD	6.55	123.74	112.60
1	Y	24	ARG	N-CA-C	6.54	118.49	111.36
1	Y	1	PRO	N-CA-CB	-6.54	95.81	103.00
1	P	34	LEU	O-C-N	-6.52	115.21	122.12
1	R	23	GLY	CA-C-O	-6.51	115.21	122.24
1	R	32	THR	CA-CB-OG1	-6.51	99.84	109.60
1	Q	110	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	H	110	ARG	NH1-CZ-NH2	-6.50	110.85	119.30
1	I	121	GLY	O-C-N	6.50	131.09	123.62
1	H	29	ASP	CB-CA-C	-6.50	100.42	110.81
1	P	22	PHE	N-CA-C	6.49	121.49	113.50
1	K	11	VAL	O-C-N	-6.49	115.14	121.83
1	T	98	VAL	CA-C-O	6.49	127.94	120.67
1	E	41	LEU	O-C-N	-6.49	114.28	122.26
1	Q	112	GLN	CG-CD-NE2	6.48	126.12	116.40
1	D	13	ARG	NE-CZ-NH2	6.46	125.01	119.20
1	O	140	SER	O-C-N	-6.46	113.84	122.43
1	U	86	ASP	CA-C-N	6.46	128.83	120.44
1	U	86	ASP	C-N-CA	6.46	128.83	120.44
1	N	52	HIS	CA-CB-CG	-6.45	107.35	113.80
1	N	98	VAL	N-CA-C	6.45	117.41	108.12
1	Q	87	ALA	CA-C-O	-6.45	113.58	120.42
1	J	25	GLN	N-CA-C	6.44	119.24	110.55
1	R	77	LEU	CA-C-N	6.44	129.20	120.38
1	R	77	LEU	C-N-CA	6.44	129.20	120.38
1	L	34	LEU	CA-C-O	-6.43	113.60	120.42
1	G	104	TYR	CA-C-O	6.43	127.27	119.49
1	G	111	HIS	CE1-NE2-CD2	-6.43	102.57	109.00
1	A	6	LEU	CA-C-O	-6.42	113.25	120.32
1	V	80	TYR	CA-CB-CG	6.42	125.46	113.90
1	Y	25	GLN	N-CA-C	6.42	118.61	110.33
1	H	11	VAL	CA-C-O	-6.41	113.55	120.47
1	I	103	LEU	CA-C-N	6.41	130.85	120.60
1	I	103	LEU	C-N-CA	6.41	130.85	120.60
1	X	86	ASP	OD1-CG-OD2	-6.41	107.53	122.90
1	N	13	ARG	NE-CZ-NH1	-6.40	115.10	121.50
1	P	112	GLN	OE1-CD-NE2	-6.40	116.20	122.60
1	U	79	HIS	CA-CB-CG	-6.39	107.41	113.80
1	U	80	TYR	CA-CB-CG	6.39	125.40	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ALA	CA-C-O	-6.39	113.05	120.20
1	L	111	HIS	CA-C-O	-6.39	110.75	119.12
1	A	102	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	J	69	GLY	CA-C-O	-6.38	115.36	121.49
1	Q	98	VAL	O-C-N	-6.38	115.97	123.05
1	O	17	ARG	O-C-N	-6.37	117.68	123.41
1	I	2	HIS	CA-CB-CG	6.37	120.17	113.80
1	F	55	ASP	CA-CB-CG	6.37	118.97	112.60
1	B	4	LEU	CB-CA-C	-6.36	99.26	109.75
1	D	85	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	P	42	HIS	CA-C-O	6.36	128.84	121.28
1	T	132	LYS	CA-C-O	6.36	127.29	120.55
1	X	2	HIS	N-CA-C	6.35	118.75	108.34
1	X	112	GLN	CG-CD-NE2	6.35	125.92	116.40
1	X	2	HIS	O-C-N	-6.34	115.85	123.27
1	K	135	VAL	CA-C-O	-6.34	114.45	121.05
1	I	69	GLY	CA-C-O	-6.34	115.41	121.49
1	L	114	VAL	CA-C-O	-6.34	111.34	119.39
1	T	22	PHE	N-CA-C	6.34	121.09	113.23
1	R	41	LEU	O-C-N	-6.33	114.17	122.59
1	V	36	GLN	OE1-CD-NE2	-6.33	116.27	122.60
1	K	100	LEU	CA-C-O	-6.32	113.78	120.55
1	A	85	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	L	133	LEU	CA-C-O	-6.32	113.81	120.63
1	B	93	LEU	CA-C-N	6.31	126.64	119.83
1	B	93	LEU	C-N-CA	6.31	126.64	119.83
1	H	139	LEU	CA-C-O	-6.31	114.20	120.82
1	L	34	LEU	O-C-N	6.31	129.34	122.15
1	E	32	THR	CA-C-O	-6.30	114.20	120.82
1	O	58	ASP	O-C-N	-6.30	115.53	122.09
1	C	12	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	O	63	ALA	CA-C-N	6.29	129.57	120.38
1	O	63	ALA	C-N-CA	6.29	129.57	120.38
1	L	85	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	J	140	SER	CA-C-O	-6.28	111.89	119.49
1	L	52	HIS	CA-CB-CG	-6.28	107.52	113.80
1	B	32	THR	CA-CB-OG1	-6.27	100.19	109.60
1	I	34	LEU	O-C-N	-6.27	114.03	122.43
1	T	112	GLN	CG-CD-NE2	6.26	125.80	116.40
1	A	136	ARG	NE-CZ-NH2	6.26	124.83	119.20
1	I	85	ARG	CD-NE-CZ	6.26	133.17	124.40
1	D	114	VAL	O-C-N	6.26	128.95	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	7	ASN	OD1-CG-ND2	-6.25	116.34	122.60
1	S	9	PRO	N-CA-CB	6.25	108.75	103.25
1	I	112	GLN	CG-CD-NE2	6.25	125.77	116.40
1	N	40	ALA	N-CA-C	6.23	118.88	111.71
1	C	87	ALA	CA-C-N	6.22	128.98	120.46
1	C	87	ALA	C-N-CA	6.22	128.98	120.46
1	E	63	ALA	CA-C-N	6.21	128.89	120.38
1	E	63	ALA	C-N-CA	6.21	128.89	120.38
1	J	80	TYR	CA-CB-CG	6.21	125.08	113.90
1	A	112	GLN	CG-CD-NE2	6.20	125.71	116.40
1	S	79	HIS	CA-CB-CG	-6.19	107.61	113.80
1	H	110	ARG	NE-CZ-NH1	6.19	127.69	121.50
1	J	35	PHE	CA-C-O	-6.18	114.33	120.70
1	N	58	ASP	O-C-N	-6.18	115.66	122.09
1	D	41	LEU	CA-C-O	6.18	126.77	119.48
1	S	55	ASP	CA-CB-CG	6.17	118.77	112.60
1	K	137	TYR	CA-C-O	6.17	127.30	120.82
1	S	18	GLU	CA-C-O	6.17	125.56	119.51
1	H	52	HIS	CA-CB-CG	-6.17	107.63	113.80
1	I	17	ARG	N-CA-C	6.17	117.93	109.18
1	B	11	VAL	CA-C-N	6.16	130.46	120.60
1	B	11	VAL	C-N-CA	6.16	130.46	120.60
1	L	55	ASP	CA-C-O	-6.16	112.88	119.97
1	Q	73	ASN	OD1-CG-ND2	6.16	128.76	122.60
1	L	70	ILE	CB-CG1-CD1	6.16	126.74	113.80
1	R	54	GLY	CA-C-O	-6.16	114.40	120.75
1	J	99	HIS	CA-CB-CG	-6.16	107.64	113.80
1	O	18	GLU	CA-C-N	6.15	126.27	119.87
1	O	18	GLU	C-N-CA	6.15	126.27	119.87
1	A	98	VAL	N-CA-C	6.15	116.98	108.12
1	M	71	VAL	N-CA-CB	6.15	118.41	111.21
1	M	79	HIS	CB-CG-ND1	6.15	131.93	122.70
1	O	99	HIS	CA-CB-CG	-6.15	107.65	113.80
1	M	97	GLU	CA-C-N	-6.14	114.40	122.94
1	M	97	GLU	C-N-CA	-6.14	114.40	122.94
1	A	106	ARG	CD-NE-CZ	6.14	133.00	124.40
1	U	91	ILE	O-C-N	-6.14	116.40	122.97
1	G	23	GLY	N-CA-C	6.13	127.72	113.18
1	G	86	ASP	CA-C-N	6.13	128.41	120.44
1	G	86	ASP	C-N-CA	6.13	128.41	120.44
1	P	130	GLY	O-C-N	-6.13	116.22	122.17
1	C	36	GLN	N-CA-C	-6.13	104.52	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	V	138	LEU	CA-C-N	6.12	128.49	120.28
1	V	138	LEU	C-N-CA	6.12	128.49	120.28
1	J	85	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	F	135	VAL	O-C-N	6.12	127.80	121.87
1	G	53	GLU	O-C-N	-6.11	115.73	122.09
1	I	18	GLU	N-CA-C	6.11	123.32	109.81
1	Y	79	HIS	ND1-CE1-NE2	6.11	114.51	108.40
1	O	131	TYR	CA-C-O	6.11	127.03	120.55
1	A	103	LEU	CA-C-N	6.11	130.92	120.72
1	A	103	LEU	C-N-CA	6.11	130.92	120.72
1	N	100	LEU	CA-C-O	-6.11	114.41	120.70
1	P	74	PRO	CA-C-O	-6.10	111.54	118.98
1	G	7	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	M	85	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	Q	24	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	J	63	ALA	CA-C-N	6.10	128.74	120.38
1	J	63	ALA	C-N-CA	6.10	128.74	120.38
1	P	17	ARG	NE-CZ-NH2	6.09	124.68	119.20
1	O	81	SER	O-C-N	-6.09	114.50	122.59
1	K	35	PHE	O-C-N	-6.08	115.80	122.07
1	F	37	PHE	CA-CB-CG	6.08	119.88	113.80
1	Y	90	SER	O-C-N	6.08	129.63	122.34
1	Y	129	GLU	CA-C-N	6.08	126.84	120.03
1	Y	129	GLU	C-N-CA	6.08	126.84	120.03
1	U	112	GLN	CG-CD-NE2	6.08	125.51	116.40
1	J	100	LEU	N-CA-C	6.07	117.97	111.36
1	N	6	LEU	CA-C-O	-6.07	113.64	120.32
1	M	58	ASP	CA-CB-CG	6.07	118.67	112.60
1	Q	42	HIS	CA-C-O	-6.07	113.29	120.57
1	Q	111	HIS	CA-CB-CG	6.06	119.86	113.80
1	V	120	LYS	CB-CG-CD	-6.06	97.35	111.30
1	N	53	GLU	CA-C-N	6.06	126.71	119.98
1	N	53	GLU	C-N-CA	6.06	126.71	119.98
1	S	41	LEU	CA-C-O	6.06	126.44	119.35
1	Y	4	LEU	CA-C-O	-6.06	113.83	120.43
1	R	75	GLY	CA-C-O	6.06	130.32	122.33
1	X	106	ARG	CD-NE-CZ	6.05	132.88	124.40
1	J	99	HIS	CA-C-O	-6.04	113.61	120.32
1	S	119	ALA	O-C-N	-6.04	114.70	122.20
1	L	25	GLN	CA-CB-CG	6.04	126.17	114.10
1	O	31	GLU	CA-CB-CG	6.04	126.17	114.10
1	L	113	SER	CA-CB-OG	6.03	123.16	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	24	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	O	42	HIS	CA-C-N	6.03	130.41	122.51
1	O	42	HIS	C-N-CA	6.03	130.41	122.51
1	H	122	GLN	CB-CG-CD	6.03	122.85	112.60
1	G	112[A]	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	G	112[B]	GLN	OE1-CD-NE2	6.02	128.62	122.60
1	K	35	PHE	CB-CA-C	6.02	120.33	110.88
1	U	87	ALA	CA-C-O	-6.02	114.50	120.82
1	Y	38	ALA	N-CA-C	6.01	117.92	111.36
1	C	42	HIS	CA-CB-CG	-6.01	107.79	113.80
1	D	140	SER	CA-C-O	-6.00	113.48	120.20
1	E	73	ASN	OD1-CG-ND2	6.00	128.60	122.60
1	N	1	PRO	CA-N-CD	-6.00	103.61	112.00
1	K	7	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	U	42	HIS	N-CA-CB	5.99	121.01	111.91
1	M	14	LEU	CA-C-N	5.99	132.88	122.05
1	M	14	LEU	C-N-CA	5.99	132.88	122.05
1	R	43	ILE	CA-C-O	5.99	129.00	121.40
1	L	23	GLY	CA-C-N	5.98	132.96	121.54
1	L	23	GLY	C-N-CA	5.98	132.96	121.54
1	H	130	GLY	CA-C-O	-5.98	114.94	120.80
1	P	29	ASP	CA-CB-CG	5.98	118.58	112.60
1	Q	115	ILE	CA-C-O	5.97	126.19	119.92
1	Q	137	TYR	O-C-N	-5.97	115.79	122.12
1	S	107	GLU	O-C-N	-5.97	115.17	122.82
1	U	22	PHE	N-CA-C	5.97	121.48	113.72
1	L	23	GLY	N-CA-C	5.97	127.32	113.18
1	V	98	VAL	O-C-N	-5.96	116.72	123.10
1	R	77	LEU	O-C-N	-5.96	114.59	122.33
1	M	108	GLU	O-C-N	-5.95	115.82	122.12
1	L	37	PHE	CA-C-O	5.94	127.06	120.82
1	A	15	GLY	O-C-N	-5.94	114.98	122.70
1	E	15	GLY	O-C-N	-5.94	114.98	122.70
1	P	118	VAL	N-CA-C	-5.94	106.96	113.43
1	H	139	LEU	N-CA-CB	5.93	118.61	110.01
1	B	86	ASP	CA-C-O	-5.93	113.40	120.10
1	C	94	PRO	CA-C-N	5.93	130.91	123.14
1	C	94	PRO	C-N-CA	5.93	130.91	123.14
1	F	139	LEU	CA-C-O	-5.93	113.56	120.20
1	N	115	ILE	CA-C-O	5.93	126.15	119.92
1	T	129	GLU	CA-C-N	5.93	126.67	120.03
1	T	129	GLU	C-N-CA	5.93	126.67	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	13	ARG	O-C-N	-5.93	114.19	122.37
1	Y	27	LEU	O-C-N	-5.92	115.29	122.22
1	H	54	GLY	CA-C-O	-5.92	114.65	120.75
1	K	51	ASN	CA-C-N	5.92	130.29	122.30
1	K	51	ASN	C-N-CA	5.92	130.29	122.30
1	M	32	THR	CA-CB-OG1	-5.92	100.73	109.60
1	J	124	VAL	CA-C-O	-5.91	114.05	120.67
1	Y	72	LEU	CA-C-N	5.91	131.81	123.30
1	Y	72	LEU	C-N-CA	5.91	131.81	123.30
1	C	122	GLN	CB-CG-CD	5.91	122.65	112.60
1	C	87	ALA	O-C-N	-5.91	115.99	122.07
1	F	135	VAL	CA-C-O	-5.90	114.81	120.95
1	Y	11	VAL	CA-C-N	5.90	130.04	120.60
1	Y	11	VAL	C-N-CA	5.90	130.04	120.60
1	O	17	ARG	N-CA-C	5.90	117.44	108.07
1	M	98	VAL	O-C-N	-5.90	116.79	123.10
1	Q	24	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	F	17	ARG	CA-CB-CG	5.89	125.88	114.10
1	M	63	ALA	O-C-N	-5.89	115.88	122.12
1	A	85	ARG	NH1-CZ-NH2	5.88	126.94	119.30
1	I	17	ARG	O-C-N	-5.88	114.63	122.74
1	N	126	LEU	CA-C-O	-5.88	112.78	119.78
1	Y	99	HIS	CA-CB-CG	-5.88	107.92	113.80
1	S	63	ALA	CA-C-N	5.88	128.43	120.38
1	S	63	ALA	C-N-CA	5.88	128.43	120.38
1	A	136	ARG	CD-NE-CZ	5.87	132.62	124.40
1	X	139	LEU	N-CA-CB	5.87	118.69	109.94
1	D	96	VAL	CA-C-O	-5.87	114.25	120.53
1	G	55	ASP	CA-CB-CG	5.87	118.47	112.60
1	E	107	GLU	CA-C-N	5.87	128.73	120.28
1	E	107	GLU	C-N-CA	5.87	128.73	120.28
1	R	40	ALA	O-C-N	-5.87	115.04	122.43
1	S	99	HIS	CA-CB-CG	-5.87	107.93	113.80
1	E	28	THR	O-C-N	5.87	128.11	122.07
1	A	110	ARG	CD-NE-CZ	5.86	132.61	124.40
1	G	12	ASN	OD1-CG-ND2	-5.86	116.74	122.60
1	H	124	VAL	O-C-N	-5.86	116.83	123.10
1	A	79	HIS	CA-CB-CG	-5.86	107.94	113.80
1	P	53	GLU	CG-CD-OE2	5.86	131.87	118.40
1	R	11	VAL	CA-C-N	5.86	129.97	120.60
1	R	11	VAL	C-N-CA	5.86	129.97	120.60
1	X	25	GLN	OE1-CD-NE2	5.85	128.45	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	7	ASN	CA-C-N	5.85	131.06	121.87
1	R	7	ASN	C-N-CA	5.85	131.06	121.87
1	X	53	GLU	OE1-CD-OE2	-5.85	108.86	122.90
1	Y	51	ASN	CB-CG-ND2	5.85	125.18	116.40
1	P	53	GLU	CA-C-N	5.85	126.47	119.98
1	P	53	GLU	C-N-CA	5.85	126.47	119.98
1	R	11	VAL	CA-C-O	-5.85	114.15	120.47
1	X	67	TYR	CA-C-N	-5.85	113.42	122.49
1	X	67	TYR	C-N-CA	-5.85	113.42	122.49
1	P	43	ILE	O-C-N	-5.84	116.75	123.00
1	I	76	ALA	CA-C-N	5.84	128.69	120.28
1	I	76	ALA	C-N-CA	5.84	128.69	120.28
1	V	88	VAL	CA-C-O	5.84	127.03	120.95
1	O	25	GLN	CA-C-O	5.84	128.64	121.87
1	L	100	LEU	N-CA-C	5.83	117.71	111.36
1	J	24	ARG	CA-C-O	5.83	126.53	119.31
1	N	26	THR	CB-CA-C	-5.83	100.37	110.45
1	R	69	GLY	O-C-N	-5.83	117.99	123.87
1	J	120	LYS	O-C-N	5.82	128.38	122.09
1	A	69	GLY	CA-C-N	5.82	131.19	122.75
1	A	69	GLY	C-N-CA	5.82	131.19	122.75
1	I	44	GLN	OE1-CD-NE2	5.82	128.42	122.60
1	M	31	GLU	CA-CB-CG	5.82	125.73	114.10
1	M	79	HIS	CE1-NE2-CD2	-5.82	103.18	109.00
1	P	1	PRO	CA-N-CD	-5.81	103.86	112.00
1	F	24	ARG	CA-C-O	5.81	126.88	120.90
1	L	21	VAL	CA-C-O	5.81	128.04	120.78
1	A	86	ASP	CA-C-N	5.81	127.99	120.44
1	A	86	ASP	C-N-CA	5.81	127.99	120.44
1	X	139	LEU	CB-CA-C	-5.81	101.52	110.81
1	Q	57	ILE	CA-C-N	5.80	127.99	120.44
1	Q	57	ILE	C-N-CA	5.80	127.99	120.44
1	D	108	GLU	CA-C-N	5.80	129.88	120.60
1	D	108	GLU	C-N-CA	5.80	129.88	120.60
1	R	112	GLN	CG-CD-NE2	5.80	125.10	116.40
1	Q	13	ARG	NE-CZ-NH2	5.79	124.42	119.20
1	J	41	LEU	CA-C-O	5.79	126.07	119.18
1	C	139	LEU	N-CA-CB	5.79	118.40	110.01
1	O	19	PRO	N-CA-C	5.79	121.15	114.03
1	L	63	ALA	CA-C-O	5.78	126.54	120.42
1	P	32	THR	CA-CB-OG1	-5.77	100.94	109.60
1	T	81	SER	N-CA-C	5.77	119.08	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	SER	CA-C-N	5.77	131.85	122.39
1	D	16	SER	C-N-CA	5.77	131.85	122.39
1	Y	108	GLU	N-CA-C	5.77	118.34	111.71
1	E	21	VAL	CA-C-O	5.77	126.27	120.73
1	L	106	ARG	NE-CZ-NH2	5.76	124.39	119.20
1	C	24	ARG	CA-C-O	5.76	125.72	119.15
1	F	80	TYR	CA-C-O	-5.76	112.27	120.51
1	N	99	HIS	CA-CB-CG	-5.76	108.04	113.80
1	C	22	PHE	N-CA-C	5.76	121.21	113.72
1	C	56	LEU	O-C-N	5.76	128.00	122.07
1	K	129	GLU	CA-C-O	5.75	126.60	120.10
1	C	120	LYS	CA-C-N	-5.75	113.49	120.51
1	C	120	LYS	C-N-CA	-5.75	113.49	120.51
1	R	139	LEU	N-CA-C	-5.75	104.92	111.07
1	I	51	ASN	OD1-CG-ND2	-5.75	116.85	122.60
1	M	38	ALA	N-CA-C	5.75	117.62	111.36
1	J	31	GLU	CA-C-O	5.75	126.64	120.55
1	T	102	ASN	CA-C-N	5.74	128.24	120.38
1	T	102	ASN	C-N-CA	5.74	128.24	120.38
1	B	60	ILE	O-C-N	-5.74	116.29	121.91
1	M	42	HIS	CB-CA-C	-5.74	102.50	111.39
1	X	79	HIS	CA-CB-CG	-5.74	108.06	113.80
1	U	40	ALA	CA-C-O	-5.74	113.37	119.97
1	B	107	GLU	CA-C-N	5.74	128.24	120.38
1	B	107	GLU	C-N-CA	5.74	128.24	120.38
1	T	112	GLN	OE1-CD-NE2	-5.74	116.86	122.60
1	X	103	LEU	O-C-N	-5.73	116.05	122.12
1	X	41	LEU	CA-C-N	5.73	130.95	122.82
1	X	41	LEU	C-N-CA	5.73	130.95	122.82
1	Y	139	LEU	N-CA-CB	5.73	118.54	110.12
1	E	28	THR	CA-C-O	-5.72	114.81	120.82
1	J	7	ASN	O-C-N	5.72	130.10	123.30
1	N	126	LEU	O-C-N	5.72	129.38	122.35
1	O	131	TYR	CA-C-N	5.72	128.21	120.44
1	O	131	TYR	C-N-CA	5.72	128.21	120.44
1	H	5	ILE	CA-C-O	-5.71	114.18	120.97
1	M	27	LEU	CA-C-O	5.70	126.59	120.55
1	M	100	LEU	CA-C-O	-5.70	114.45	120.55
1	M	129	GLU	CA-C-N	5.70	126.42	120.03
1	M	129	GLU	C-N-CA	5.70	126.42	120.03
1	J	43	ILE	CA-C-O	-5.70	115.98	121.63
1	S	107	GLU	CA-C-O	5.70	127.60	121.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	29	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	35	PHE	CA-CB-CG	-5.70	108.10	113.80
1	B	63	ALA	CA-C-N	5.70	128.18	120.38
1	B	63	ALA	C-N-CA	5.70	128.18	120.38
1	D	102	ASN	CA-CB-CG	-5.70	106.90	112.60
1	E	20[A]	GLU	CA-C-O	5.70	126.52	119.97
1	E	20[B]	GLU	CA-C-O	5.70	126.52	119.97
1	G	111	HIS	CG-CD2-NE2	5.69	112.89	107.20
1	T	31	GLU	CB-CG-CD	5.69	122.28	112.60
1	M	51	ASN	OD1-CG-ND2	5.69	128.29	122.60
1	Y	9	PRO	CA-C-N	5.69	132.41	121.54
1	Y	9	PRO	C-N-CA	5.69	132.41	121.54
1	F	5	ILE	CA-C-O	-5.69	113.30	120.86
1	H	72	LEU	CA-C-O	-5.69	114.22	120.30
1	M	63	ALA	CA-C-O	5.69	126.58	120.55
1	A	4	LEU	CA-C-N	5.69	131.06	123.10
1	A	4	LEU	C-N-CA	5.69	131.06	123.10
1	S	112	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	X	92	SER	CA-C-O	-5.68	112.63	119.27
1	C	35	PHE	CA-C-N	5.68	128.16	120.44
1	C	35	PHE	C-N-CA	5.68	128.16	120.44
1	B	123	ILE	O-C-N	-5.67	117.28	123.18
1	B	140	SER	CB-CA-C	-5.67	100.13	110.63
1	A	17	ARG	CD-NE-CZ	5.67	132.34	124.40
1	F	56	LEU	CA-C-O	-5.67	114.86	120.70
1	G	63	ALA	CA-C-N	5.67	128.66	120.38
1	G	63	ALA	C-N-CA	5.67	128.66	120.38
1	S	28	THR	CA-C-O	-5.67	114.87	120.82
1	C	85	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	K	12	ASN	O-C-N	-5.66	115.75	122.20
1	R	36	GLN	CA-C-O	-5.66	114.55	120.55
1	N	127	GLY	CA-C-O	-5.66	114.86	122.33
1	B	99	HIS	CA-CB-CG	-5.65	108.15	113.80
1	C	141	GLN	CA-C-O	-5.65	111.19	120.80
1	F	24	ARG	CA-C-N	5.65	132.33	121.54
1	F	24	ARG	C-N-CA	5.65	132.33	121.54
1	Y	112	GLN	OE1-CD-NE2	-5.65	116.95	122.60
1	L	39	GLU	CA-C-O	-5.65	114.53	120.63
1	K	99	HIS	CG-CD2-NE2	5.64	112.84	107.20
1	T	97	GLU	O-C-N	-5.64	116.78	123.22
1	M	24	ARG	CG-CD-NE	5.64	124.41	112.00
1	V	115	ILE	CB-CA-C	-5.64	104.68	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	63	ALA	CA-C-O	5.63	126.45	119.97
1	X	86	ASP	CB-CG-OD1	5.63	131.35	118.40
1	D	5	ILE	CA-C-O	-5.63	114.27	120.97
1	F	17	ARG	N-CA-C	5.63	117.35	108.96
1	U	63	ALA	CA-C-N	5.63	128.09	120.38
1	U	63	ALA	C-N-CA	5.63	128.09	120.38
1	N	137	TYR	O-C-N	5.62	128.56	122.15
1	X	38	ALA	CA-C-O	5.62	126.72	120.82
1	C	73	ASN	CA-C-O	5.62	126.17	120.38
1	B	112	GLN	CG-CD-NE2	5.62	124.82	116.40
1	U	51	ASN	OD1-CG-ND2	-5.61	116.99	122.60
1	F	63	ALA	CA-C-N	5.61	128.57	120.38
1	F	63	ALA	C-N-CA	5.61	128.57	120.38
1	K	112	GLN	CG-CD-NE2	5.61	124.82	116.40
1	Q	58	ASP	CA-CB-CG	5.61	118.21	112.60
1	N	2	HIS	CA-C-O	5.61	126.19	120.24
1	Y	112	GLN	CG-CD-NE2	5.61	124.81	116.40
1	J	9	PRO	O-C-N	-5.60	116.25	123.03
1	X	33	ASP	CA-CB-CG	-5.60	107.00	112.60
1	U	18	GLU	CA-C-N	5.60	125.12	119.19
1	U	18	GLU	C-N-CA	5.60	125.12	119.19
1	J	96	VAL	N-CA-CB	5.60	118.92	111.64
1	H	80	TYR	CA-C-N	-5.59	113.39	122.34
1	H	80	TYR	C-N-CA	-5.59	113.39	122.34
1	U	36	GLN	OE1-CD-NE2	-5.59	117.00	122.60
1	G	139	LEU	O-C-N	-5.59	115.68	122.22
1	B	24	ARG	N-CA-C	5.59	118.10	111.33
1	O	100	LEU	CA-C-O	-5.59	115.14	120.90
1	R	4	LEU	CA-C-N	5.59	129.88	122.95
1	R	4	LEU	C-N-CA	5.59	129.88	122.95
1	E	51	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	I	84	ILE	CA-C-O	-5.59	114.92	120.85
1	I	17	ARG	CD-NE-CZ	5.59	132.22	124.40
1	D	39	GLU	CA-C-O	-5.59	114.66	120.92
1	O	110	ARG	CA-C-O	-5.58	111.81	119.12
1	K	113	SER	CA-C-N	-5.58	113.49	121.52
1	K	113	SER	C-N-CA	-5.58	113.49	121.52
1	S	86	ASP	O-C-N	-5.58	115.41	122.27
1	C	106	ARG	CA-C-O	-5.57	114.86	120.77
1	O	102	ASN	CA-C-N	5.57	128.01	120.38
1	O	102	ASN	C-N-CA	5.57	128.01	120.38
1	X	112	GLN	O-C-N	-5.57	116.80	123.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	19	PRO	CA-C-O	5.57	124.67	118.38
1	K	112	GLN	CA-C-N	5.56	130.67	123.00
1	K	112	GLN	C-N-CA	5.56	130.67	123.00
1	G	36	GLN	CG-CD-NE2	5.55	124.73	116.40
1	J	71	VAL	N-CA-C	-5.55	98.45	107.28
1	R	82	TYR	N-CA-CB	5.55	119.61	110.39
1	T	94	PRO	CB-CA-C	-5.55	104.74	111.46
1	B	35	PHE	N-CA-CB	5.55	118.28	110.12
1	L	84	ILE	O-C-N	5.55	127.55	121.83
1	Y	42	HIS	N-CA-C	5.55	119.63	112.86
1	C	98	VAL	N-CA-C	5.55	116.47	108.48
1	N	36	GLN	OE1-CD-NE2	-5.55	117.05	122.60
1	T	36	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	K	89	SER	CB-CA-C	-5.54	100.38	110.63
1	G	93	LEU	CA-C-N	5.54	125.71	119.90
1	G	93	LEU	C-N-CA	5.54	125.71	119.90
1	P	132	LYS	O-C-N	5.53	128.06	122.09
1	A	17	ARG	N-CA-C	5.53	116.37	108.74
1	I	23	GLY	N-CA-C	-5.53	105.72	112.68
1	X	80	TYR	CA-CB-CG	5.53	123.85	113.90
1	H	77	LEU	O-C-N	-5.53	115.03	122.43
1	R	82	TYR	N-CA-C	-5.53	105.80	112.54
1	U	18	GLU	N-CA-C	5.53	122.02	109.81
1	O	112	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	B	39	GLU	O-C-N	5.52	128.45	122.15
1	J	98	VAL	O-C-N	-5.52	117.11	123.07
1	B	60	ILE	CA-C-N	5.52	127.68	120.28
1	B	60	ILE	C-N-CA	5.52	127.68	120.28
1	H	26	THR	N-CA-C	-5.52	103.62	110.41
1	J	115	ILE	CA-C-O	5.52	125.72	119.92
1	A	33	ASP	CB-CA-C	-5.52	101.63	110.79
1	B	9	PRO	N-CA-CB	5.51	108.10	103.25
1	Q	136	ARG	O-C-N	-5.51	116.28	122.12
1	L	72	LEU	CA-C-O	5.50	126.30	120.36
1	U	129	GLU	CA-C-O	5.50	126.15	119.49
1	A	86	ASP	O-C-N	-5.50	116.29	122.12
1	V	140	SER	CA-C-O	-5.50	111.90	119.05
1	F	67	TYR	CA-C-O	-5.49	115.20	121.68
1	L	45	LEU	CA-C-O	-5.49	114.34	120.66
1	S	29	ASP	CB-CA-C	-5.49	102.02	110.81
1	A	58	ASP	CA-CB-CG	5.49	118.09	112.60
1	F	57	ILE	O-C-N	5.49	127.19	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	115	ILE	CA-C-N	5.48	126.58	120.06
1	H	115	ILE	C-N-CA	5.48	126.58	120.06
1	K	99	HIS	CA-CB-CG	-5.48	108.32	113.80
1	G	96	VAL	N-CA-CB	5.48	119.27	111.82
1	M	112	GLN	CG-CD-NE2	5.47	124.61	116.40
1	Q	42	HIS	ND1-CE1-NE2	5.47	113.87	108.40
1	C	71	VAL	N-CA-C	-5.46	99.88	107.80
1	G	79	HIS	CA-CB-CG	-5.46	108.33	113.80
1	M	85	ARG	O-C-N	-5.46	116.35	122.03
1	C	28	THR	CB-CA-C	5.46	119.86	110.79
1	K	7	ASN	CB-CG-OD1	5.46	131.72	120.80
1	K	78	SER	CB-CA-C	-5.46	101.40	110.68
1	B	17	ARG	CA-C-N	5.46	135.11	121.80
1	B	17	ARG	C-N-CA	5.46	135.11	121.80
1	G	10	ASN	CA-CB-CG	-5.45	107.15	112.60
1	Q	99	HIS	CA-C-N	5.45	127.85	120.44
1	Q	99	HIS	C-N-CA	5.45	127.85	120.44
1	D	86	ASP	O-C-N	-5.45	115.85	122.22
1	H	47	PHE	CA-CB-CG	-5.45	108.36	113.80
1	O	102	ASN	CA-CB-CG	-5.45	107.15	112.60
1	T	8	GLY	CA-C-N	5.44	125.37	119.76
1	T	8	GLY	C-N-CA	5.44	125.37	119.76
1	J	69	GLY	O-C-N	5.44	129.37	123.87
1	K	113	SER	CA-C-O	5.44	126.31	120.38
1	Q	39	GLU	N-CA-C	-5.44	105.04	110.97
1	O	38	ALA	CA-C-O	5.44	126.19	120.42
1	S	80	TYR	CA-CB-CG	5.44	123.69	113.90
1	B	31	GLU	CB-CG-CD	5.43	121.84	112.60
1	M	79	HIS	ND1-CE1-NE2	5.43	113.83	108.40
1	Q	9	PRO	CB-CA-C	-5.43	104.45	111.46
1	F	72	LEU	CA-C-N	5.43	130.43	122.66
1	F	72	LEU	C-N-CA	5.43	130.43	122.66
1	T	136	ARG	NH1-CZ-NH2	5.43	126.36	119.30
1	Q	129	GLU	CA-C-O	5.43	126.28	120.20
1	U	30	ILE	CB-CG1-CD1	5.43	125.20	113.80
1	A	53	GLU	CA-C-N	5.43	126.00	119.98
1	A	53	GLU	C-N-CA	5.43	126.00	119.98
1	X	42	HIS	CA-C-N	5.43	130.40	122.69
1	X	42	HIS	C-N-CA	5.43	130.40	122.69
1	D	36	GLN	CA-C-N	5.42	127.82	120.44
1	D	36	GLN	C-N-CA	5.42	127.82	120.44
1	L	17	ARG	CG-CD-NE	5.42	123.92	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	120	LYS	CA-C-O	5.42	126.16	120.42
1	K	9	PRO	CA-C-O	5.42	127.48	121.36
1	H	42	HIS	N-CA-C	5.41	119.05	111.74
1	H	54	GLY	O-C-N	5.41	127.39	122.19
1	E	18	GLU	CA-C-O	5.41	124.30	119.59
1	I	116	ALA	O-C-N	-5.41	115.10	121.32
1	R	104	TYR	O-C-N	-5.41	115.36	122.39
1	P	42	HIS	CA-CB-CG	-5.41	108.39	113.80
1	J	31	GLU	N-CA-CB	-5.41	102.17	110.12
1	R	52	HIS	CA-C-N	5.41	127.84	120.54
1	R	52	HIS	C-N-CA	5.41	127.84	120.54
1	K	84	ILE	O-C-N	-5.40	115.69	121.80
1	R	34	LEU	O-C-N	-5.40	115.62	122.27
1	V	6	LEU	CA-C-O	-5.40	114.58	120.36
1	S	112	GLN	CG-CD-NE2	5.40	124.50	116.40
1	S	120	LYS	CA-CB-CG	-5.40	103.31	114.10
1	U	11	VAL	O-C-N	-5.39	115.70	121.80
1	X	25	GLN	N-CA-CB	-5.39	101.34	110.50
1	P	129	GLU	CB-CG-CD	5.39	121.76	112.60
1	H	2	HIS	CA-C-O	5.38	126.14	120.33
1	J	36	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	I	9	PRO	N-CA-CB	5.38	108.10	103.31
1	U	16	SER	N-CA-C	5.38	122.25	110.80
1	K	16	SER	CA-C-O	5.37	126.15	119.97
1	J	7	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	P	44	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	C	107	GLU	CA-C-O	5.36	127.09	121.19
1	X	41	LEU	N-CA-C	-5.36	106.11	113.30
1	M	53	GLU	O-C-N	-5.36	116.52	122.09
1	N	70	ILE	CB-CG1-CD1	5.36	125.06	113.80
1	V	115	ILE	N-CA-C	5.36	116.84	111.00
1	L	21	VAL	CA-C-N	5.36	131.78	121.54
1	L	21	VAL	C-N-CA	5.36	131.78	121.54
1	M	123	ILE	CA-C-N	-5.36	115.49	122.94
1	M	123	ILE	C-N-CA	-5.36	115.49	122.94
1	R	139	LEU	N-CA-CB	5.36	117.78	110.01
1	T	80	TYR	CA-CB-CG	5.35	123.54	113.90
1	A	119	ALA	O-C-N	5.35	128.94	122.68
1	B	28	THR	CA-C-O	5.35	126.21	120.70
1	A	25	GLN	CA-CB-CG	5.35	124.80	114.10
1	L	82	TYR	CB-CG-CD2	5.35	128.82	120.80
1	N	12	ASN	OD1-CG-ND2	-5.35	117.25	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	HIS	O-C-N	-5.34	117.07	123.27
1	Y	10	ASN	OD1-CG-ND2	5.34	127.94	122.60
1	D	127	GLY	CA-C-O	5.34	129.55	122.39
1	P	36	GLN	CB-CA-C	-5.34	102.49	110.88
1	A	120	LYS	CB-CG-CD	-5.34	99.02	111.30
1	A	83	ALA	N-CA-CB	5.33	118.55	110.28
1	B	15	GLY	CA-C-O	5.33	124.66	119.27
1	N	31	GLU	CB-CG-CD	5.33	121.67	112.60
1	S	134	ALA	N-CA-CB	5.33	118.05	110.16
1	X	124	VAL	CA-C-O	-5.33	114.70	120.67
1	C	72	LEU	N-CA-C	5.33	117.10	108.41
1	E	112	GLN	CG-CD-NE2	5.33	124.39	116.40
1	J	42	HIS	O-C-N	-5.33	116.57	122.91
1	E	70	ILE	CB-CG1-CD1	5.33	124.99	113.80
1	Q	90	SER	CA-CB-OG	-5.32	100.45	111.10
1	M	35	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	43	ILE	CA-C-O	-5.32	116.14	121.45
1	B	120	LYS	CB-CG-CD	-5.31	99.08	111.30
1	M	107	GLU	CA-C-N	5.31	127.66	120.38
1	M	107	GLU	C-N-CA	5.31	127.66	120.38
1	T	86	ASP	CA-CB-CG	5.31	117.91	112.60
1	X	10	ASN	O-C-N	-5.31	115.53	122.59
1	C	57	ILE	CA-C-N	5.31	127.70	120.54
1	C	57	ILE	C-N-CA	5.31	127.70	120.54
1	J	129	GLU	CA-C-N	5.31	125.97	120.03
1	J	129	GLU	C-N-CA	5.31	125.97	120.03
1	L	55	ASP	CA-CB-CG	5.31	117.91	112.60
1	P	30	ILE	CB-CA-C	-5.31	104.98	112.14
1	Y	99	HIS	CA-C-O	-5.30	114.56	120.66
1	G	113	SER	CA-C-O	-5.30	114.49	120.32
1	A	22	PHE	CA-CB-CG	5.30	119.10	113.80
1	U	39	GLU	O-C-N	5.30	127.74	122.12
1	G	104	TYR	O-C-N	-5.30	115.50	122.39
1	J	139	LEU	CA-C-O	5.29	126.16	120.55
1	C	107	GLU	CA-C-N	5.29	127.63	120.38
1	C	107	GLU	C-N-CA	5.29	127.63	120.38
1	M	27	LEU	O-C-N	-5.29	116.51	122.12
1	U	38	ALA	CB-CA-C	-5.29	102.54	110.90
1	L	112[A]	GLN	CG-CD-NE2	5.29	124.33	116.40
1	L	112[B]	GLN	CG-CD-NE2	5.29	124.33	116.40
1	V	10	ASN	O-C-N	-5.29	115.56	122.59
1	A	89	SER	CB-CA-C	-5.28	99.28	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	44	GLN	OE1-CD-NE2	5.28	127.88	122.60
1	N	91	ILE	CA-C-O	-5.28	116.13	121.67
1	E	34	LEU	CA-C-N	5.28	127.35	120.28
1	E	34	LEU	C-N-CA	5.28	127.35	120.28
1	G	80	TYR	CA-CB-CG	5.28	123.39	113.90
1	K	38	ALA	N-CA-C	5.28	118.18	111.69
1	U	129	GLU	O-C-N	-5.28	115.53	122.39
1	J	10	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	N	70	ILE	CA-CB-CG1	5.27	119.36	110.40
1	U	136	ARG	NE-CZ-NH1	-5.26	116.23	121.50
1	Y	8	GLY	CA-C-N	5.26	125.27	119.90
1	Y	8	GLY	C-N-CA	5.26	125.27	119.90
1	E	31	GLU	CA-CB-CG	5.26	124.62	114.10
1	E	133	LEU	CA-C-N	5.26	127.60	120.44
1	E	133	LEU	C-N-CA	5.26	127.60	120.44
1	L	54	GLY	CA-C-O	-5.26	115.33	120.75
1	A	55	ASP	N-CA-CB	5.26	117.94	110.16
1	D	106	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	S	141	GLN	CB-CG-CD	-5.25	103.67	112.60
1	F	106	ARG	CA-C-O	-5.25	115.20	120.77
1	O	106	ARG	NE-CZ-NH1	5.25	126.75	121.50
1	K	63	ALA	CA-C-N	5.25	128.04	120.38
1	K	63	ALA	C-N-CA	5.25	128.04	120.38
1	T	36	GLN	CG-CD-NE2	5.25	124.27	116.40
1	V	141	GLN	N-CA-C	5.25	125.70	111.00
1	T	115	ILE	CA-C-O	5.25	125.43	119.92
1	L	88	VAL	CA-C-N	5.24	127.83	120.28
1	L	88	VAL	C-N-CA	5.24	127.83	120.28
1	K	72	LEU	CA-C-N	5.24	130.84	123.30
1	K	72	LEU	C-N-CA	5.24	130.84	123.30
1	G	139	LEU	N-CA-CB	5.24	118.28	110.22
1	L	107	GLU	CA-C-N	5.23	127.55	120.38
1	L	107	GLU	C-N-CA	5.23	127.55	120.38
1	A	2	HIS	N-CA-C	5.23	116.94	108.41
1	X	53	GLU	CA-C-N	5.23	125.79	119.98
1	X	53	GLU	C-N-CA	5.23	125.79	119.98
1	L	139	LEU	N-CA-CB	5.23	117.90	110.16
1	H	109	PHE	CA-CB-CG	5.23	119.03	113.80
1	Q	35	PHE	CA-C-O	-5.23	115.31	120.90
1	D	32	THR	N-CA-CB	-5.23	102.44	110.12
1	X	71	VAL	N-CA-C	-5.22	100.22	107.80
1	E	134	ALA	O-C-N	5.22	127.73	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	29	ASP	CB-CA-C	-5.22	102.46	110.81
1	J	5	ILE	CA-C-O	-5.22	114.55	120.66
1	L	99	HIS	CA-CB-CG	-5.22	108.58	113.80
1	M	44	GLN	OE1-CD-NE2	5.22	127.82	122.60
1	P	141	GLN	CA-C-O	5.21	129.66	120.80
1	D	107	GLU	CA-C-N	5.21	127.52	120.38
1	D	107	GLU	C-N-CA	5.21	127.52	120.38
1	X	116	ALA	N-CA-C	5.21	120.69	113.45
1	X	42	HIS	CA-C-O	5.21	128.31	122.27
1	S	20	GLU	N-CA-C	-5.20	106.08	112.90
1	Y	30	ILE	CB-CA-C	-5.20	105.31	111.97
1	A	26	THR	N-CA-CB	5.20	118.45	110.70
1	K	58	ASP	CA-CB-CG	5.20	117.80	112.60
1	P	23	GLY	CA-C-O	-5.20	118.84	122.22
1	R	140	SER	CA-C-N	5.20	131.06	121.70
1	R	140	SER	C-N-CA	5.20	131.06	121.70
1	T	119	ALA	CA-C-O	-5.20	115.53	121.82
1	S	128	ALA	O-C-N	-5.20	116.28	122.20
1	K	136	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	H	135	VAL	CA-C-O	-5.19	115.55	120.95
1	I	87	ALA	CA-C-N	5.19	127.57	120.46
1	I	87	ALA	C-N-CA	5.19	127.57	120.46
1	H	18	GLU	N-CA-C	5.19	121.27	109.81
1	T	25	GLN	N-CA-C	5.18	117.95	110.28
1	V	36	GLN	CB-CA-C	5.18	119.10	110.81
1	Y	57	ILE	CA-C-N	5.18	127.17	120.44
1	Y	57	ILE	C-N-CA	5.18	127.17	120.44
1	J	49	GLN	CA-CB-CG	5.18	124.45	114.10
1	H	124	VAL	N-CA-C	5.17	116.17	108.46
1	E	24	ARG	CA-C-N	5.17	129.61	120.87
1	E	24	ARG	C-N-CA	5.17	129.61	120.87
1	N	32	THR	CA-CB-OG1	-5.17	101.84	109.60
1	R	33	ASP	N-CA-CB	5.17	118.29	110.28
1	C	63	ALA	CA-C-N	5.17	127.46	120.38
1	C	63	ALA	C-N-CA	5.17	127.46	120.38
1	H	17	ARG	O-C-N	-5.17	117.89	123.42
1	R	63	ALA	CA-C-N	5.17	127.93	120.38
1	R	63	ALA	C-N-CA	5.17	127.93	120.38
1	V	132	LYS	CA-C-O	5.17	126.02	120.70
1	N	41	LEU	CA-C-O	5.17	125.68	119.43
1	Y	110	ARG	NH1-CZ-NH2	-5.16	112.59	119.30
1	Q	38	ALA	CB-CA-C	-5.16	102.07	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	77	LEU	N-CA-C	-5.16	105.78	111.71
1	P	80	TYR	CA-CB-CG	5.16	123.19	113.90
1	O	87	ALA	O-C-N	-5.16	116.76	122.07
1	S	141	GLN	CG-CD-OE1	-5.16	110.48	120.80
1	Y	96	VAL	CA-CB-CG1	5.16	119.17	110.40
1	J	33	ASP	CA-CB-CG	-5.16	107.44	112.60
1	H	99	HIS	CA-CB-CG	-5.15	108.65	113.80
1	H	140	SER	CA-C-O	-5.15	112.61	119.10
1	F	5	ILE	N-CA-CB	5.15	118.16	111.83
1	G	90	SER	CA-CB-OG	-5.15	100.81	111.10
1	J	41	LEU	N-CA-C	-5.15	107.00	113.28
1	L	29	ASP	CA-CB-CG	5.15	117.75	112.60
1	T	67	TYR	CA-C-N	-5.14	114.58	122.60
1	T	67	TYR	C-N-CA	-5.14	114.58	122.60
1	C	16	SER	N-CA-C	5.14	119.04	112.87
1	C	112	GLN	CG-CD-NE2	5.14	124.11	116.40
1	H	7	ASN	CB-CG-OD1	5.14	131.08	120.80
1	V	63	ALA	CA-C-N	5.14	127.42	120.38
1	V	63	ALA	C-N-CA	5.14	127.42	120.38
1	K	102	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	K	137	TYR	O-C-N	-5.14	116.78	122.07
1	M	37	PHE	N-CA-CB	5.13	117.46	110.01
1	O	45	LEU	CA-C-O	-5.13	114.76	120.66
1	N	9	PRO	N-CA-CB	5.13	107.88	103.31
1	Y	43	ILE	N-CA-C	5.13	116.25	108.96
1	I	101	SER	CA-CB-OG	-5.13	100.85	111.10
1	O	95	VAL	O-C-N	-5.13	117.64	123.18
1	H	129	GLU	CA-C-N	5.12	125.77	120.03
1	H	129	GLU	C-N-CA	5.12	125.77	120.03
1	I	101	SER	CA-C-O	5.12	127.83	121.94
1	S	38	ALA	O-C-N	5.12	127.35	122.07
1	Y	29	ASP	O-C-N	-5.12	116.76	122.09
1	A	76	ALA	CA-C-N	5.12	128.80	120.60
1	A	76	ALA	C-N-CA	5.12	128.80	120.60
1	E	79	HIS	CA-CB-CG	-5.12	108.68	113.80
1	P	106	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	N	102	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	O	85	ARG	CD-NE-CZ	5.12	131.56	124.40
1	Y	100	LEU	O-C-N	5.12	128.36	122.17
1	F	119	ALA	CA-C-N	-5.11	113.03	120.29
1	F	119	ALA	C-N-CA	-5.11	113.03	120.29
1	U	25	GLN	N-CA-C	-5.11	103.65	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	13	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	70	ILE	CA-C-O	5.11	126.00	120.43
1	I	71	VAL	N-CA-C	-5.11	100.29	107.75
1	C	18	GLU	CA-C-N	5.10	124.76	119.56
1	C	18	GLU	C-N-CA	5.10	124.76	119.56
1	N	60	ILE	N-CA-C	-5.10	105.57	110.72
1	G	107	GLU	CA-C-N	5.10	127.37	120.38
1	G	107	GLU	C-N-CA	5.10	127.37	120.38
1	I	70	ILE	O-C-N	-5.10	117.54	123.00
1	D	41	LEU	N-CA-C	-5.09	105.76	112.94
1	E	98	VAL	N-CA-CB	-5.09	103.09	111.44
1	F	141	GLN	CB-CG-CD	5.09	121.25	112.60
1	P	7	ASN	CA-CB-CG	-5.09	107.51	112.60
1	C	17	ARG	CD-NE-CZ	-5.09	117.27	124.40
1	X	60	ILE	O-C-N	-5.09	116.61	121.90
1	N	42	HIS	CB-CG-CD2	-5.09	124.58	131.20
1	O	107	GLU	CA-C-N	5.09	127.10	120.28
1	O	107	GLU	C-N-CA	5.09	127.10	120.28
1	V	94	PRO	CA-C-O	5.09	126.92	120.97
1	L	94	PRO	N-CA-CB	5.09	107.84	103.36
1	D	53	GLU	CA-C-O	5.08	126.34	120.90
1	H	106	ARG	O-C-N	-5.08	117.25	122.84
1	D	127	GLY	CA-C-N	5.08	128.03	120.31
1	D	127	GLY	C-N-CA	5.08	128.03	120.31
1	H	107	GLU	CA-C-N	5.08	127.08	120.28
1	H	107	GLU	C-N-CA	5.08	127.08	120.28
1	K	37	PHE	N-CA-C	-5.08	105.83	111.36
1	C	88	VAL	CA-C-O	5.08	126.23	120.95
1	Y	9	PRO	N-CA-CB	5.08	107.72	103.25
1	C	106	ARG	CB-CG-CD	5.07	122.97	111.30
1	H	86	ASP	CA-C-N	5.07	127.04	120.44
1	H	86	ASP	C-N-CA	5.07	127.04	120.44
1	U	67	TYR	CA-C-N	-5.07	114.63	122.49
1	U	67	TYR	C-N-CA	-5.07	114.63	122.49
1	H	23	GLY	CA-C-O	-5.07	117.32	122.59
1	P	112	GLN	CG-CD-NE2	5.07	124.00	116.40
1	R	73	ASN	O-C-N	5.07	126.20	120.83
1	G	129	GLU	O-C-N	-5.06	116.43	122.20
1	B	42	HIS	CB-CA-C	-5.06	104.70	111.89
1	D	35	PHE	CA-C-O	5.05	126.13	120.82
1	R	106	ARG	O-C-N	-5.05	117.28	122.84
1	S	89	SER	CA-CB-OG	-5.05	100.99	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	GLU	N-CA-C	-5.05	106.97	113.23
1	A	102	ASN	CA-C-N	5.05	127.30	120.38
1	A	102	ASN	C-N-CA	5.05	127.30	120.38
1	G	129	GLU	CA-C-O	5.05	125.86	120.20
1	I	119	ALA	O-C-N	-5.05	116.77	122.68
1	U	90	SER	CA-CB-OG	-5.05	101.00	111.10
1	C	10	ASN	CA-C-N	5.05	128.58	120.30
1	C	10	ASN	C-N-CA	5.05	128.58	120.30
1	K	31	GLU	N-CA-CB	-5.05	102.70	110.12
1	R	107	GLU	CA-C-O	5.05	126.89	121.44
1	O	80	TYR	CA-CB-CG	5.04	122.98	113.90
1	R	115	ILE	CA-C-N	5.04	126.06	120.06
1	R	115	ILE	C-N-CA	5.04	126.06	120.06
1	T	71	VAL	N-CA-C	-5.04	100.48	107.80
1	K	37	PHE	N-CA-CB	5.04	117.62	110.16
1	L	79	HIS	CA-CB-CG	-5.04	108.76	113.80
1	M	122	GLN	N-CA-C	5.04	117.38	108.75
1	N	67	TYR	CA-C-O	-5.04	115.73	121.68
1	Q	37	PHE	N-CA-C	-5.04	105.97	111.82
1	O	96	VAL	CA-C-N	5.04	129.03	121.72
1	O	96	VAL	C-N-CA	5.04	129.03	121.72
1	X	136	ARG	CD-NE-CZ	5.04	131.45	124.40
1	K	9	PRO	O-C-N	-5.03	116.50	122.89
1	K	116	ALA	N-CA-C	5.03	120.52	113.57
1	L	17	ARG	NH1-CZ-NH2	-5.03	112.75	119.30
1	V	79	HIS	CA-CB-CG	-5.03	108.77	113.80
1	E	25	GLN	N-CA-C	5.03	117.02	110.43
1	U	77	LEU	CA-C-N	5.03	127.27	120.38
1	U	77	LEU	C-N-CA	5.03	127.27	120.38
1	X	102	ASN	CA-C-N	5.03	127.27	120.38
1	X	102	ASN	C-N-CA	5.03	127.27	120.38
1	V	11	VAL	CA-C-O	5.03	125.90	120.47
1	J	21	VAL	N-CA-C	5.03	115.25	110.53
1	C	22	PHE	CB-CA-C	-5.02	101.11	109.55
1	G	118	VAL	CB-CA-C	-5.02	104.97	111.20
1	T	58	ASP	CA-CB-CG	5.02	117.62	112.60
1	J	2	HIS	CA-CB-CG	5.02	118.82	113.80
1	P	55	ASP	CA-CB-CG	5.02	117.62	112.60
1	Q	36	GLN	CA-C-O	5.02	125.77	120.10
1	D	52	HIS	CA-CB-CG	-5.02	108.78	113.80
1	D	40	ALA	N-CA-C	5.02	119.03	113.01
1	Q	63	ALA	CA-C-N	5.02	127.70	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	63	ALA	C-N-CA	5.02	127.70	120.38
1	E	38	ALA	CA-C-O	-5.01	115.54	120.70
1	Y	53	GLU	OE1-CD-OE2	-5.01	110.88	122.90
1	E	74	PRO	CA-C-O	-5.01	112.87	118.98
1	H	122	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	F	86	ASP	O-C-N	-5.01	116.11	122.27
1	E	7	ASN	CA-C-N	-5.01	114.01	121.87
1	E	7	ASN	C-N-CA	-5.01	114.01	121.87
1	F	98	VAL	CA-C-O	5.00	126.28	120.67

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	141	GLN	Mainchain
1	H	40	ALA	Mainchain
1	I	115	ILE	Mainchain
1	K	12	ASN	Mainchain
1	R	111	HIS	Mainchain
1	X	109	PHE	Mainchain

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	1094	0	1059	31	0
1	B	1105	0	1065	28	0
1	C	1093	0	1064	23	0
1	D	1094	0	1059	22	0
1	E	1108	0	1078	27	0
1	F	1107	0	1076	19	0
1	G	1101	0	1067	21	0
1	H	1096	0	1062	31	0
1	I	1090	0	1055	33	0
1	J	1093	0	1064	23	0
1	K	1051	0	1021	17	0
1	L	1085	0	1050	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1098	0	1069	24	0
1	N	1028	0	1006	15	0
1	O	1096	0	1066	24	0
1	P	1099	0	1071	26	0
1	Q	1109	0	1086	19	0
1	R	1094	0	1055	24	0
1	S	1108	0	1084	25	0
1	T	1104	0	1076	17	0
1	U	1093	0	1064	37	0
1	V	1056	0	1034	22	0
1	X	1034	0	1012	15	0
1	Y	1096	0	1062	28	0
2	A	18	0	24	5	0
2	B	18	0	24	5	0
2	C	18	0	24	7	0
2	D	18	0	23	5	0
2	E	17	0	21	3	0
2	F	17	0	20	3	0
2	G	18	0	24	6	0
2	H	18	0	24	5	0
2	I	18	0	24	4	0
2	J	18	0	24	2	0
2	K	18	0	24	6	0
2	L	18	0	23	7	0
2	M	18	0	24	3	0
2	N	18	0	23	3	0
2	O	18	0	24	8	0
2	P	18	0	24	7	0
2	Q	18	0	24	11	0
2	R	18	0	24	6	0
2	S	18	0	24	8	0
2	T	18	0	24	4	0
2	U	18	0	24	8	0
2	V	18	0	24	5	0
2	X	18	0	23	3	0
2	Y	18	0	24	7	0
3	A	90	0	0	14	0
3	B	98	0	0	10	0
3	C	100	0	0	12	0
3	D	96	0	0	6	0
3	E	93	0	0	10	0
3	F	91	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	91	0	0	9	0
3	H	75	0	0	12	0
3	I	91	0	0	8	0
3	J	91	0	0	10	0
3	K	83	0	0	2	0
3	L	86	0	0	8	0
3	M	97	0	0	8	0
3	N	96	0	0	7	0
3	O	89	0	0	9	0
3	P	97	0	0	10	0
3	Q	97	0	0	9	0
3	R	103	0	0	13	0
3	S	84	0	0	10	0
3	T	87	0	0	8	0
3	U	101	0	0	13	0
3	V	107	0	0	9	0
3	X	79	0	0	10	0
3	Y	80	0	0	12	0
All	All	28764	0	25970	600	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 11.

All (600) 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:N:141:GLN:HA	1:N:142:GLN:N	1.42	1.23
1:F:142:GLN:N	3:F:2084:HOH:O	1.69	1.20
1:U:140:SER:O	1:U:142:GLN:N	1.81	1.13
1:U:117:PRO:HG3	2:U:151:GOL:H11	1.36	1.06
1:M:14:LEU:HD13	2:M:152:GOL:H11	1.38	1.04
1:N:141:GLN:CA	1:N:142:GLN:N	2.15	0.99
1:C:141:GLN:HE21	1:C:142:GLN:N	1.60	0.98
1:D:112[B]:GLN:HG3	2:D:151:GOL:H31	1.49	0.93
1:G:112[B]:GLN:HG3	2:G:151:GOL:H2	1.49	0.93
1:K:1:PRO:H2	1:K:43:ILE:HG22	1.35	0.92
3:F:2067:HOH:O	2:H:151:GOL:H2	1.67	0.92
1:M:98:VAL:HG13	3:M:2086:HOH:O	1.71	0.90
1:F:98:VAL:HG13	3:F:2075:HOH:O	1.73	0.89
1:U:112:GLN:HG3	3:U:2099:HOH:O	1.73	0.87
1:Q:14:LEU:HD13	2:Q:152:GOL:H2	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:PRO:HG2	1:H:43:ILE:HG22	1.57	0.86
1:X:98:VAL:HG13	3:X:2065:HOH:O	1.75	0.86
1:C:98:VAL:HG13	3:C:2088:HOH:O	1.74	0.86
1:E:123:ILE:HG22	3:E:2083:HOH:O	1.74	0.85
1:R:113:SER:HB2	3:R:2084:HOH:O	1.75	0.85
1:A:98:VAL:HG13	3:A:2077:HOH:O	1.77	0.84
1:U:43:ILE:HG21	1:U:139:LEU:HD11	1.59	0.84
1:D:62:GLU:OE1	1:Q:22:PHE:HA	1.78	0.83
1:I:113:SER:HB2	3:I:2073:HOH:O	1.77	0.83
1:P:132:LYS:HG3	3:P:2085:HOH:O	1.78	0.82
1:L:123:ILE:HG22	3:L:2080:HOH:O	1.80	0.82
1:J:98:VAL:HG13	3:J:2080:HOH:O	1.78	0.82
1:H:132:LYS:HG3	3:H:2068:HOH:O	1.77	0.81
1:U:80:TYR:HB2	3:U:2053:HOH:O	1.80	0.81
1:L:20:GLU:HA	1:L:23:GLY:HA2	1.60	0.81
1:Q:123:ILE:HG22	3:Q:2083:HOH:O	1.77	0.81
1:K:14:LEU:HD13	2:K:152:GOL:H2	1.61	0.81
1:E:141:GLN:CB	1:E:142:GLN:N	2.18	0.80
1:F:113:SER:HA	3:F:2044:HOH:O	1.80	0.80
1:G:141:GLN:CA	1:G:142:GLN:N	2.31	0.80
1:Y:79:HIS:HE1	3:Y:2059:HOH:O	1.64	0.80
1:J:141:GLN:HB3	1:J:142:GLN:N	1.97	0.80
1:D:98:VAL:HG13	3:D:2085:HOH:O	1.82	0.79
1:T:1:PRO:HD2	1:T:43:ILE:HG22	1.63	0.79
1:P:98:VAL:HG13	3:P:2081:HOH:O	1.83	0.79
1:K:141:GLN:NE2	1:K:142:GLN:N	2.31	0.78
1:B:14:LEU:HA	2:B:152:GOL:H11	1.64	0.78
1:I:80:TYR:HB2	3:I:2041:HOH:O	1.82	0.78
1:B:80:TYR:HB2	3:B:2044:HOH:O	1.82	0.78
1:I:141:GLN:NE2	1:I:142:GLN:N	2.31	0.78
1:U:117:PRO:CG	2:U:151:GOL:H11	2.15	0.77
1:A:53:GLU:HB3	3:A:2035:HOH:O	1.85	0.77
1:A:80:TYR:HB2	3:A:2049:HOH:O	1.84	0.76
1:L:117:PRO:HG3	2:L:151:GOL:H12	1.65	0.76
1:H:40:ALA:C	1:H:42:HIS:H	1.93	0.76
1:G:141:GLN:HA	1:G:142:GLN:N	2.01	0.76
1:H:141:GLN:O	1:H:142:GLN:N	2.04	0.76
1:C:103:LEU:HB2	3:C:2068:HOH:O	1.85	0.75
1:R:117:PRO:HG3	2:R:151:GOL:H11	1.67	0.75
1:M:41:LEU:O	1:M:42:HIS:HB2	1.85	0.75
1:P:112:GLN:HG3	3:P:2072:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:100:LEU:HD23	3:P:2087:HOH:O	1.86	0.74
1:S:80:TYR:HB2	3:S:2043:HOH:O	1.87	0.74
1:O:133:LEU:HD23	3:O:2083:HOH:O	1.87	0.74
1:V:112:GLN:HG3	3:V:2086:HOH:O	1.88	0.74
1:F:112[B]:GLN:HB2	3:F:2089:HOH:O	1.87	0.74
1:B:116:ALA:HB3	3:B:2098:HOH:O	1.88	0.74
1:M:1:PRO:HG2	1:M:43:ILE:HG22	1.69	0.73
1:A:133:LEU:HD23	3:A:2085:HOH:O	1.88	0.73
1:U:24:ARG:HA	3:U:2014:HOH:O	1.87	0.73
1:J:53:GLU:HB3	3:J:2037:HOH:O	1.88	0.73
1:L:80:TYR:HB2	3:L:2043:HOH:O	1.89	0.72
1:A:25:GLN:HG3	3:A:2008:HOH:O	1.89	0.72
1:Y:103:LEU:HD13	3:Y:2059:HOH:O	1.87	0.72
1:D:105:ALA:HB2	3:D:2063:HOH:O	1.90	0.72
1:F:112[A]:GLN:HB2	3:F:2089:HOH:O	1.88	0.72
1:A:4:LEU:HD13	3:A:2001:HOH:O	1.90	0.71
1:T:113:SER:O	2:T:151:GOL:H12	1.90	0.71
1:T:98:VAL:HG13	3:T:2074:HOH:O	1.91	0.71
1:S:113:SER:HB2	3:S:2073:HOH:O	1.90	0.71
1:A:6:LEU:HB2	3:A:2001:HOH:O	1.89	0.70
1:A:70:ILE:HG23	3:A:2001:HOH:O	1.89	0.70
1:F:113:SER:O	2:F:151:GOL:H11	1.92	0.70
1:P:34:LEU:HG	3:P:2015:HOH:O	1.91	0.70
1:N:117:PRO:HG2	3:N:2093:HOH:O	1.90	0.70
1:E:141:GLN:HB3	1:E:142:GLN:N	2.05	0.69
1:P:132:LYS:HD3	3:P:2025:HOH:O	1.91	0.69
1:D:17:ARG:HG2	1:D:17:ARG:HH11	1.58	0.69
1:E:113:SER:HB2	3:E:2080:HOH:O	1.91	0.69
1:M:88:VAL:HG12	3:M:2077:HOH:O	1.92	0.69
1:N:112:GLN:HG3	3:N:2090:HOH:O	1.93	0.69
1:N:14:LEU:HD13	2:N:152:GOL:H31	1.74	0.68
2:U:151:GOL:H12	3:U:2081:HOH:O	1.93	0.68
1:S:1:PRO:HA	3:S:2001:HOH:O	1.93	0.68
1:U:113:SER:O	2:U:151:GOL:H12	1.93	0.68
1:Y:117:PRO:HG3	2:Y:151:GOL:H12	1.74	0.68
1:D:112[B]:GLN:HG3	2:D:151:GOL:C3	2.24	0.68
1:N:113:SER:O	2:N:151:GOL:H31	1.94	0.67
2:Q:151:GOL:C1	1:Y:111:HIS:HB3	2.24	0.67
1:U:79:HIS:HE1	3:U:2079:HOH:O	1.75	0.67
1:T:1:PRO:HD2	1:T:43:ILE:CG2	2.24	0.67
1:F:79:HIS:ND1	3:F:2044:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:PHE:HA	3:G:2023:HOH:O	1.94	0.66
1:H:22:PHE:HA	3:H:2004:HOH:O	1.95	0.66
1:I:140:SER:O	1:I:142:GLN:N	2.30	0.66
1:T:14:LEU:HA	2:T:152:GOL:H11	1.78	0.66
1:J:80:TYR:HB2	3:J:2050:HOH:O	1.94	0.65
1:Y:14:LEU:HA	2:Y:152:GOL:H11	1.77	0.65
1:P:112:GLN:HB2	2:P:151:GOL:H31	1.78	0.65
1:X:103:LEU:HD12	3:X:2064:HOH:O	1.97	0.65
1:D:21:VAL:HG12	1:D:101:SER:HB2	1.78	0.65
1:Q:112:GLN:HG3	3:Q:2093:HOH:O	1.97	0.65
1:V:25:GLN:HE21	1:V:30:ILE:CG1	2.10	0.65
1:B:112:GLN:HB2	2:B:151:GOL:O2	1.97	0.64
1:V:53:GLU:HB2	3:X:2025:HOH:O	1.96	0.64
1:O:10:ASN:O	2:O:152:GOL:H2	1.97	0.64
1:I:111:HIS:ND1	2:K:151:GOL:H2	2.13	0.64
1:B:15:GLY:HA2	3:B:2011:HOH:O	1.98	0.63
1:G:103:LEU:HD12	3:G:2079:HOH:O	1.96	0.63
1:H:132:LYS:HB3	3:H:2071:HOH:O	1.97	0.63
2:Q:151:GOL:H11	1:Y:111:HIS:CG	2.33	0.63
1:H:88:VAL:HG12	3:H:2058:HOH:O	1.98	0.63
1:H:43:ILE:HG21	1:H:139:LEU:HD21	1.81	0.63
3:N:2072:HOH:O	2:S:151:GOL:H2	1.99	0.63
1:R:40:ALA:C	1:R:42:HIS:H	2.05	0.63
1:K:141:GLN:CD	1:K:142:GLN:N	2.42	0.62
1:U:105:ALA:HB2	3:U:2066:HOH:O	1.98	0.62
2:Y:151:GOL:H31	3:Y:2038:HOH:O	1.98	0.62
1:E:31:GLU:HB2	3:E:2016:HOH:O	1.99	0.62
2:S:150:GOL:H11	2:S:152:GOL:H31	1.80	0.62
1:A:141:GLN:NE2	1:A:142:GLN:N	2.47	0.62
1:I:1:PRO:HG2	1:I:43:ILE:HG22	1.81	0.62
1:B:132:LYS:HG3	3:B:2088:HOH:O	2.00	0.62
1:G:112[B]:GLN:HG2	1:G:113:SER:N	2.14	0.62
1:I:14:LEU:HD13	2:I:152:GOL:H32	1.79	0.62
2:B:151:GOL:H2	3:G:2071:HOH:O	1.98	0.62
1:R:1:PRO:HD2	1:R:43:ILE:HG22	1.81	0.61
1:A:141:GLN:CD	1:A:142:GLN:N	2.58	0.61
2:Q:151:GOL:H11	1:Y:111:HIS:HB3	1.82	0.61
1:M:111:HIS:ND1	2:P:151:GOL:O2	2.34	0.61
1:B:142:GLN:N	1:B:143:GLY:O	2.33	0.61
1:X:89:SER:HA	3:X:2042:HOH:O	2.00	0.61
1:B:43:ILE:HG21	1:B:139:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2090:HOH:O	1:J:136:ARG:HB3	2.00	0.61
1:H:22:PHE:CE2	2:H:152:GOL:H12	2.36	0.60
1:M:72:LEU:HG	1:M:74:PRO:HD3	1.83	0.60
1:C:88:VAL:HG12	3:C:2081:HOH:O	2.01	0.60
1:K:38:ALA:HB1	1:K:43:ILE:O	2.02	0.60
1:S:22:PHE:CE2	2:S:152:GOL:H32	2.35	0.60
1:B:30:ILE:HG22	1:B:34:LEU:HD12	1.83	0.60
1:I:113:SER:HB2	3:I:2074:HOH:O	2.01	0.60
2:P:151:GOL:H2	3:P:2095:HOH:O	2.01	0.60
3:C:2077:HOH:O	2:J:151:GOL:H2	2.01	0.60
1:F:112[B]:GLN:HG3	2:F:151:GOL:O2	2.02	0.60
1:I:38:ALA:HB1	1:I:43:ILE:O	2.02	0.60
1:P:1:PRO:CG	1:P:43:ILE:HG22	2.31	0.60
1:D:46:THR:HG21	1:Q:20:GLU:OE2	2.03	0.59
1:G:20:GLU:OE1	1:G:21:VAL:HG23	2.03	0.59
1:C:141:GLN:NE2	1:C:142:GLN:N	2.41	0.59
1:B:20:GLU:OE1	1:B:21:VAL:HG23	2.02	0.59
1:I:14:LEU:HA	2:I:152:GOL:H11	1.85	0.59
1:F:1:PRO:HD2	1:F:43:ILE:HG22	1.85	0.58
1:V:112:GLN:HA	3:V:2087:HOH:O	2.03	0.58
1:B:1:PRO:HD2	1:B:43:ILE:HG22	1.84	0.58
1:D:112[B]:GLN:CG	2:D:151:GOL:H31	2.28	0.58
1:O:112:GLN:HG3	3:O:2070:HOH:O	2.02	0.58
1:U:17:ARG:HG2	1:U:17:ARG:HH11	1.68	0.58
1:U:103:LEU:HD13	3:U:2079:HOH:O	2.04	0.58
1:K:141:GLN:HE21	1:K:142:GLN:N	2.02	0.58
1:B:111:HIS:ND1	2:G:151:GOL:H12	2.18	0.58
2:C:151:GOL:O1	1:J:104:TYR:HB3	2.03	0.57
1:C:124:VAL:HG11	3:C:2068:HOH:O	2.03	0.57
1:K:43:ILE:HD13	1:K:139:LEU:HD11	1.87	0.57
1:H:38:ALA:HB1	1:H:43:ILE:O	2.05	0.57
1:H:23:GLY:HA3	3:H:2005:HOH:O	2.04	0.57
1:P:1:PRO:HG2	1:P:43:ILE:HG22	1.86	0.57
1:A:141:GLN:HA	1:A:142:GLN:N	2.20	0.57
1:Y:126:LEU:N	3:Y:2045:HOH:O	2.38	0.57
1:V:27:LEU:O	1:V:31:GLU:HG3	2.05	0.56
1:E:17:ARG:HA	3:E:2009:HOH:O	2.04	0.56
1:L:19:PRO:O	1:L:20:GLU:CB	2.53	0.56
1:I:141:GLN:HE22	1:I:142:GLN:N	2.03	0.56
1:O:6:LEU:HD22	1:O:56:LEU:HD22	1.86	0.56
1:O:14:LEU:HD13	2:O:152:GOL:H11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:10:ASN:O	2:Q:152:GOL:O2	2.23	0.56
1:F:111:HIS:ND1	2:H:151:GOL:H11	2.21	0.56
1:U:130:GLY:HA3	3:U:2091:HOH:O	2.05	0.56
1:K:1:PRO:N	1:K:43:ILE:HG22	2.14	0.56
1:L:53:GLU:OE2	1:L:81:SER:OG	2.22	0.56
1:X:2:HIS:HA	1:X:44:GLN:O	2.05	0.56
1:X:132:LYS:HB3	3:X:2074:HOH:O	2.05	0.56
1:A:82:TYR:CD1	3:A:2048:HOH:O	2.53	0.56
1:B:27:LEU:HG	1:B:31:GLU:OE1	2.05	0.56
1:F:38:ALA:HB1	1:F:43:ILE:HG13	1.87	0.56
1:H:1:PRO:HG2	1:H:43:ILE:CG2	2.32	0.56
1:N:10:ASN:O	2:N:152:GOL:H2	2.04	0.56
2:R:151:GOL:H31	3:R:2101:HOH:O	2.06	0.56
1:U:102:ASN:ND2	3:U:2066:HOH:O	2.39	0.56
2:L:150:GOL:H11	2:L:152:GOL:H31	1.87	0.56
1:S:2:HIS:HA	1:S:44:GLN:O	2.06	0.56
1:R:112:GLN:HG3	3:R:2077:HOH:O	2.06	0.55
1:I:81:SER:HB2	3:I:2042:HOH:O	2.06	0.55
1:H:44:GLN:HA	3:H:2015:HOH:O	2.07	0.55
1:V:17:ARG:HB3	3:V:2007:HOH:O	2.06	0.55
1:A:111:HIS:ND1	2:D:151:GOL:H11	2.22	0.55
1:O:14:LEU:HA	2:O:152:GOL:H12	1.88	0.55
1:G:17:ARG:HA	3:G:2009:HOH:O	2.07	0.55
1:U:14:LEU:HG	3:U:2015:HOH:O	2.06	0.55
2:R:151:GOL:H12	3:R:2100:HOH:O	2.06	0.55
1:H:1:PRO:CG	1:H:43:ILE:HG22	2.35	0.54
1:B:31:GLU:HG2	1:B:47:PHE:CD2	2.43	0.54
1:F:20:GLU:CD	1:F:20:GLU:H	2.15	0.54
1:R:132:LYS:HD3	3:R:2094:HOH:O	2.07	0.54
1:T:31:GLU:HG2	1:T:47:PHE:CD2	2.42	0.54
1:E:111:HIS:ND1	2:L:151:GOL:H2	2.22	0.54
1:C:17:ARG:HA	3:C:2006:HOH:O	2.08	0.54
1:Y:38:ALA:HB1	1:Y:43:ILE:O	2.08	0.54
1:D:102:ASN:ND2	3:D:2063:HOH:O	2.41	0.54
1:E:110:ARG:NH1	2:E:150:GOL:H12	2.22	0.54
2:G:152:GOL:H32	3:G:2002:HOH:O	2.08	0.54
1:J:141:GLN:OE1	1:J:142:GLN:N	2.41	0.54
1:U:17:ARG:HG2	1:U:17:ARG:NH1	2.23	0.54
1:Q:2:HIS:HA	1:Q:44:GLN:O	2.09	0.53
1:J:37:PHE:O	1:J:41:LEU:HB2	2.07	0.53
1:O:111:HIS:ND1	2:V:151:GOL:H12	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2075:HOH:O	2:G:151:GOL:H11	2.07	0.53
1:J:1:PRO:HD2	1:J:43:ILE:HG22	1.90	0.53
1:X:64:GLU:HB3	3:X:2032:HOH:O	2.07	0.53
1:X:15:GLY:O	1:X:16:SER:C	2.51	0.53
1:X:77:LEU:HD22	3:X:2026:HOH:O	2.09	0.53
1:E:117:PRO:HG3	2:E:151:GOL:H11	1.91	0.53
1:M:1:PRO:CG	1:M:43:ILE:HG22	2.37	0.53
1:Q:117:PRO:HG3	2:Q:151:GOL:O2	2.09	0.53
1:S:19:PRO:HA	1:S:23:GLY:H	1.74	0.53
1:D:48:PHE:HB2	1:Q:21:VAL:HG21	1.89	0.53
1:X:120:LYS:HE3	3:X:2060:HOH:O	2.07	0.53
1:Y:113:SER:O	2:Y:151:GOL:H32	2.08	0.53
1:E:1:PRO:HG2	1:E:43:ILE:HG21	1.90	0.53
1:P:38:ALA:HB1	1:P:43:ILE:O	2.09	0.53
2:Q:151:GOL:H11	1:Y:111:HIS:ND1	2.23	0.53
1:I:77:LEU:HA	3:I:2042:HOH:O	2.09	0.52
1:P:14:LEU:HD13	2:P:152:GOL:H32	1.90	0.52
1:D:38:ALA:O	1:D:39:GLU:C	2.51	0.52
1:F:1:PRO:CD	1:F:43:ILE:HG22	2.39	0.52
1:C:14:LEU:HD13	2:C:152:GOL:H2	1.92	0.52
1:E:141:GLN:HG2	3:E:2089:HOH:O	2.09	0.52
1:L:15:GLY:O	1:L:16:SER:C	2.52	0.52
1:B:79:HIS:CE1	3:B:2073:HOH:O	2.62	0.52
1:C:2:HIS:HA	1:C:44:GLN:O	2.08	0.52
1:E:14:LEU:HD13	2:E:152:GOL:H11	1.92	0.52
1:H:28:THR:O	1:H:29:ASP:C	2.50	0.52
1:A:19:PRO:HA	1:A:23:GLY:O	2.10	0.52
1:H:124:VAL:HG21	3:H:2042:HOH:O	2.09	0.52
1:U:31:GLU:HG2	1:U:47:PHE:CD2	2.45	0.52
1:X:13:ARG:O	1:X:16:SER:HB3	2.10	0.52
1:F:22:PHE:CE2	2:F:152:GOL:H2	2.45	0.52
1:J:79:HIS:CE1	3:J:2060:HOH:O	2.63	0.51
1:P:15:GLY:O	1:P:17:ARG:N	2.43	0.51
1:S:32:THR:HA	3:S:2018:HOH:O	2.10	0.51
1:I:34:LEU:HD11	1:I:131:TYR:HB3	1.91	0.51
1:T:19:PRO:HD3	3:T:2007:HOH:O	2.09	0.51
1:A:14:LEU:HD13	2:A:152:GOL:H2	1.91	0.51
1:K:2:HIS:HA	1:K:44:GLN:O	2.11	0.51
2:O:151:GOL:H11	1:V:111:HIS:ND1	2.25	0.51
1:C:53:GLU:HB3	3:C:2041:HOH:O	2.11	0.51
1:J:2:HIS:HA	1:J:44:GLN:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:VAL:HG12	3:J:2073:HOH:O	2.11	0.51
1:U:25:GLN:HB2	1:U:29:ASP:HB2	1.91	0.51
1:S:25:GLN:HB3	1:S:29:ASP:HB2	1.91	0.51
1:S:81:SER:HB2	3:S:2044:HOH:O	2.10	0.51
1:T:17:ARG:HA	3:T:2008:HOH:O	2.11	0.51
1:I:38:ALA:CA	1:I:43:ILE:HG13	2.41	0.51
1:O:137:TYR:CZ	1:O:141:GLN:HG3	2.46	0.51
3:S:2033:HOH:O	1:U:80:TYR:HE1	1.93	0.51
1:I:64:GLU:HB3	3:I:2034:HOH:O	2.12	0.50
1:N:33:ASP:HA	1:N:36:GLN:NE2	2.25	0.50
1:O:43:ILE:HD13	1:O:139:LEU:HD11	1.93	0.50
1:A:130:GLY:HA3	3:A:2077:HOH:O	2.12	0.50
1:E:19:PRO:HB3	1:E:24:ARG:HA	1.92	0.50
1:J:99:HIS:CE1	3:J:2060:HOH:O	2.64	0.50
1:M:80:TYR:CD2	3:N:2047:HOH:O	2.63	0.50
1:D:19:PRO:HA	1:D:23:GLY:O	2.11	0.50
1:L:113:SER:HB2	3:L:2078:HOH:O	2.12	0.50
1:P:112:GLN:CB	2:P:151:GOL:H31	2.41	0.50
1:Q:47:PHE:O	3:Q:2025:HOH:O	2.19	0.50
1:U:47:PHE:HD2	3:U:2001:HOH:O	1.95	0.50
1:V:53:GLU:OE2	1:V:81:SER:OG	2.27	0.50
3:Q:2074:HOH:O	2:Y:151:GOL:H2	2.11	0.50
2:X:150:GOL:H12	3:X:2048:HOH:O	2.10	0.50
1:J:75:GLY:HA2	3:J:2003:HOH:O	2.11	0.50
1:L:117:PRO:HG3	2:L:151:GOL:C1	2.38	0.50
2:L:150:GOL:C1	2:L:152:GOL:H31	2.42	0.50
1:J:20:GLU:H	1:J:20:GLU:CD	2.19	0.50
1:R:43:ILE:HG21	1:R:139:LEU:HD21	1.93	0.50
1:U:25:GLN:HB2	1:U:29:ASP:CB	2.42	0.50
3:E:2026:HOH:O	1:L:102:ASN:HB3	2.11	0.50
1:G:19:PRO:HB3	3:G:2012:HOH:O	2.11	0.50
1:I:53:GLU:HB3	3:I:2027:HOH:O	2.11	0.50
1:O:43:ILE:HG21	1:O:139:LEU:HD11	1.92	0.50
1:I:112:GLN:HG3	2:I:151:GOL:O3	2.12	0.50
1:U:79:HIS:CE1	3:U:2079:HOH:O	2.59	0.50
2:A:151:GOL:H11	1:D:104:TYR:CD2	2.47	0.49
1:B:30:ILE:HG22	1:B:34:LEU:CD1	2.42	0.49
1:H:6:LEU:HD22	1:H:56:LEU:HD22	1.94	0.49
1:L:103:LEU:HB2	3:L:2068:HOH:O	2.11	0.49
1:N:64:GLU:HB3	3:N:2041:HOH:O	2.11	0.49
1:V:17:ARG:HA	3:V:2008:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:VAL:HG11	1:D:106:ARG:HD2	1.93	0.49
1:U:38:ALA:O	1:U:39:GLU:C	2.56	0.49
1:A:38:ALA:O	1:A:39:GLU:C	2.53	0.49
1:B:78:SER:HA	1:B:115:ILE:HD12	1.94	0.49
1:I:29:ASP:N	1:I:29:ASP:OD1	2.45	0.49
1:U:10:ASN:O	2:U:152:GOL:H2	2.12	0.49
1:I:38:ALA:HA	1:I:43:ILE:HG13	1.94	0.49
1:L:12:ASN:HA	1:L:27:LEU:HD22	1.93	0.49
2:Y:150:GOL:H32	3:Y:2034:HOH:O	2.12	0.49
1:E:18:GLU:O	1:E:22:PHE:HB2	2.12	0.49
1:O:41:LEU:O	1:O:43:ILE:HG23	2.12	0.49
1:C:111:HIS:ND1	2:J:151:GOL:H2	2.28	0.49
1:A:36:GLN:O	1:A:37:PHE:C	2.55	0.49
1:J:7:ASN:O	1:J:49:GLN:HA	2.13	0.49
1:Y:88:VAL:HG12	3:Y:2061:HOH:O	2.13	0.49
1:P:13:ARG:O	1:P:14:LEU:C	2.56	0.48
1:V:14:LEU:HD13	2:V:152:GOL:H2	1.95	0.48
1:C:117:PRO:HG3	2:C:151:GOL:O1	2.13	0.48
1:O:126:LEU:HB3	1:V:137:TYR:CD1	2.48	0.48
1:M:38:ALA:HB1	1:M:43:ILE:HG13	1.94	0.48
2:Q:151:GOL:H11	1:Y:111:HIS:CB	2.42	0.48
1:A:82:TYR:HD1	3:A:2048:HOH:O	1.95	0.48
1:B:113:SER:HB3	3:B:2098:HOH:O	2.12	0.48
1:E:2:HIS:HA	1:E:44:GLN:O	2.13	0.48
1:E:112:GLN:HA	3:E:2091:HOH:O	2.14	0.48
1:N:114:VAL:HA	3:N:2093:HOH:O	2.14	0.48
1:S:113:SER:CB	3:S:2073:HOH:O	2.55	0.48
1:H:31:GLU:HG3	1:H:47:PHE:CE1	2.48	0.48
1:P:1:PRO:HB2	1:P:43:ILE:HG22	1.96	0.48
1:V:25:GLN:HE21	1:V:30:ILE:HG13	1.79	0.48
1:B:77:LEU:HA	3:B:2046:HOH:O	2.12	0.48
1:H:19:PRO:HA	1:H:23:GLY:O	2.14	0.48
1:O:1:PRO:HD2	1:O:43:ILE:HG22	1.95	0.48
2:P:151:GOL:H32	3:P:2096:HOH:O	2.12	0.48
1:G:116:ALA:N	1:G:117:PRO:CD	2.77	0.48
2:O:151:GOL:H11	1:V:111:HIS:CE1	2.48	0.48
1:Y:88:VAL:HG13	1:Y:95:VAL:HG21	1.96	0.48
1:K:140:SER:O	1:K:142:GLN:N	2.32	0.48
1:L:10:ASN:O	2:L:152:GOL:H12	2.14	0.48
1:V:25:GLN:HG3	1:V:30:ILE:HD11	1.95	0.48
1:Y:113:SER:HB2	3:Y:2033:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:111:HIS:ND1	2:V:151:GOL:H2	2.29	0.48
1:A:2:HIS:HA	1:A:44:GLN:O	2.14	0.47
1:H:25:GLN:HB3	1:H:29:ASP:HB2	1.95	0.47
1:U:104:TYR:CD2	2:X:151:GOL:H11	2.48	0.47
1:H:10:ASN:HB2	3:H:2001:HOH:O	2.14	0.47
1:H:22:PHE:CZ	2:H:152:GOL:H12	2.49	0.47
1:L:6:LEU:HD22	1:L:56:LEU:HD22	1.96	0.47
1:M:113:SER:HB2	3:M:2084:HOH:O	2.14	0.47
1:O:9:PRO:HA	1:O:51:ASN:OD1	2.14	0.47
1:Y:17:ARG:O	1:Y:18:GLU:C	2.57	0.47
1:C:123:ILE:HB	3:C:2088:HOH:O	2.14	0.47
1:E:99:HIS:CG	1:E:103:LEU:HD11	2.50	0.47
1:P:80:TYR:HE1	3:Q:2031:HOH:O	1.96	0.47
1:K:14:LEU:CD1	2:K:152:GOL:H2	2.37	0.47
1:O:99:HIS:CE1	3:O:2055:HOH:O	2.67	0.47
1:R:34:LEU:HG	3:R:2024:HOH:O	2.13	0.47
1:D:103:LEU:HD12	3:D:2065:HOH:O	2.15	0.47
1:L:21:VAL:O	1:L:22:PHE:CB	2.62	0.47
1:Y:43:ILE:HD12	1:Y:139:LEU:HD21	1.97	0.47
1:P:113:SER:HB2	3:P:2079:HOH:O	2.15	0.47
1:R:78:SER:HA	1:R:115:ILE:HD12	1.97	0.47
1:S:90:SER:HA	1:U:17:ARG:NH1	2.29	0.47
1:U:17:ARG:HH11	1:U:17:ARG:CG	2.27	0.47
1:B:35:PHE:HE2	3:B:2029:HOH:O	1.98	0.47
1:L:120:LYS:HA	3:L:2076:HOH:O	2.15	0.47
1:N:78:SER:HA	1:N:115:ILE:HD12	1.97	0.47
1:U:2:HIS:HE2	1:U:46:THR:HG1	1.60	0.47
1:N:6:LEU:HD13	1:N:72:LEU:HD13	1.97	0.47
1:Y:13:ARG:O	1:Y:16:SER:OG	2.31	0.47
1:Y:17:ARG:HA	3:Y:2004:HOH:O	2.14	0.47
2:C:151:GOL:H12	3:C:2098:HOH:O	2.14	0.47
1:D:113:SER:HA	3:D:2047:HOH:O	2.15	0.47
1:G:3:PHE:HE1	1:G:139:LEU:CD2	2.27	0.47
1:G:78:SER:HA	1:G:115:ILE:HD12	1.97	0.47
1:D:112[B]:GLN:HG2	1:D:113:SER:N	2.23	0.46
1:I:72:LEU:O	1:I:97:GLU:HA	2.15	0.46
1:C:17:ARG:NH1	3:C:2009:HOH:O	2.48	0.46
1:L:16:SER:O	1:L:17:ARG:HB2	2.14	0.46
2:Q:151:GOL:C1	3:Q:2094:HOH:O	2.63	0.46
1:O:103:LEU:HB2	3:O:2068:HOH:O	2.15	0.46
1:R:132:LYS:HB3	3:R:2094:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:SER:HB2	3:C:2009:HOH:O	2.16	0.46
1:D:38:ALA:HB1	1:D:43:ILE:O	2.15	0.46
1:G:77:LEU:HA	3:G:2046:HOH:O	2.14	0.46
1:S:112:GLN:HG3	2:S:151:GOL:H31	1.97	0.46
2:U:151:GOL:O2	1:X:111:HIS:ND1	2.49	0.46
1:V:84:ILE:O	1:V:85:ARG:C	2.56	0.46
1:Y:99:HIS:CE1	3:Y:2034:HOH:O	2.67	0.46
1:M:80:TYR:HD1	3:M:2021:HOH:O	1.98	0.46
1:F:18:GLU:HA	1:F:19:PRO:HD2	1.77	0.46
1:V:15:GLY:O	1:V:17:ARG:N	2.48	0.46
1:A:124:VAL:HG21	3:A:2062:HOH:O	2.15	0.46
1:M:81:SER:HB2	3:M:2051:HOH:O	2.15	0.46
1:Q:14:LEU:CD1	2:Q:152:GOL:H2	2.39	0.46
3:A:2048:HOH:O	1:C:80:TYR:CD2	2.56	0.45
1:B:26:THR:O	1:B:29:ASP:HB2	2.15	0.45
2:O:151:GOL:H32	3:O:2087:HOH:O	2.16	0.45
1:R:81:SER:HA	3:R:2040:HOH:O	2.16	0.45
1:X:113:SER:H	2:X:151:GOL:H12	1.80	0.45
1:A:36:GLN:HE21	1:A:36:GLN:HB2	1.35	0.45
1:J:123:ILE:HB	3:J:2080:HOH:O	2.15	0.45
1:Y:112:GLN:HG3	2:Y:151:GOL:O3	2.16	0.45
1:G:2:HIS:HA	1:G:44:GLN:O	2.17	0.45
1:S:77:LEU:HA	3:S:2044:HOH:O	2.16	0.45
1:T:14:LEU:CD1	2:T:152:GOL:H11	2.46	0.45
1:P:2:HIS:HA	1:P:44:GLN:O	2.17	0.45
1:C:17:ARG:HG2	1:C:17:ARG:HH11	1.81	0.45
1:I:41:LEU:O	1:I:42:HIS:HB2	2.17	0.45
1:A:64:GLU:HB3	3:A:2040:HOH:O	2.16	0.45
1:N:99:HIS:CG	1:N:103:LEU:HD11	2.52	0.45
1:S:99:HIS:CG	1:S:103:LEU:HD11	2.51	0.45
2:C:151:GOL:H31	3:J:2071:HOH:O	2.16	0.45
1:I:15:GLY:O	1:I:17:ARG:N	2.50	0.45
1:Q:41:LEU:O	1:Q:42:HIS:HB2	2.16	0.45
1:Y:2:HIS:HA	1:Y:44:GLN:O	2.16	0.45
1:C:43:ILE:HG21	1:C:139:LEU:HD21	1.99	0.45
1:Q:37:PHE:CZ	1:Q:41:LEU:HD11	2.52	0.45
1:B:32:THR:O	1:B:36:GLN:HG3	2.16	0.45
1:I:38:ALA:HB1	1:I:43:ILE:HG13	1.98	0.45
2:U:151:GOL:O2	1:X:111:HIS:CG	2.70	0.45
1:A:6:LEU:HD22	1:A:56:LEU:HD22	2.00	0.44
1:R:19:PRO:HA	1:R:23:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:HIS:CE1	1:D:110:ARG:HA	2.52	0.44
1:T:17:ARG:O	1:T:18:GLU:C	2.60	0.44
1:T:103:LEU:HD12	3:T:2054:HOH:O	2.17	0.44
2:V:152:GOL:H31	3:V:2012:HOH:O	2.17	0.44
1:M:41:LEU:O	1:M:42:HIS:CB	2.57	0.44
1:G:95:VAL:HB	3:G:2056:HOH:O	2.17	0.44
1:H:79:HIS:CE1	3:H:2038:HOH:O	2.70	0.44
1:O:111:HIS:HA	3:O:2068:HOH:O	2.17	0.44
1:Q:103:LEU:HD12	3:Q:2082:HOH:O	2.17	0.44
1:R:139:LEU:HD23	1:R:139:LEU:HA	1.84	0.44
1:B:15:GLY:O	1:B:16:SER:C	2.61	0.44
1:B:22:PHE:CE2	2:B:152:GOL:H32	2.52	0.44
1:I:13:ARG:O	1:I:15:GLY:N	2.51	0.44
1:L:2:HIS:HA	1:L:44:GLN:O	2.17	0.44
1:M:1:PRO:HG2	1:M:43:ILE:CG2	2.45	0.44
2:Q:151:GOL:H12	3:Q:2094:HOH:O	2.17	0.44
1:S:31:GLU:HB2	3:S:2017:HOH:O	2.18	0.44
2:V:151:GOL:H32	3:V:2062:HOH:O	2.18	0.44
1:X:130:GLY:HA3	3:X:2065:HOH:O	2.16	0.44
1:C:2:HIS:HE2	1:C:46:THR:HG1	1.66	0.44
1:T:25:GLN:HB2	3:T:2011:HOH:O	2.18	0.44
1:A:113:SER:O	2:A:151:GOL:H12	2.18	0.44
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.62	0.43
1:P:74:PRO:HG2	1:P:78:SER:HB2	2.00	0.43
1:Q:137:TYR:CD2	1:Q:137:TYR:C	2.96	0.43
1:Q:139:LEU:HD23	1:Q:139:LEU:HA	1.79	0.43
1:V:28:THR:O	1:V:29:ASP:C	2.60	0.43
1:Y:78:SER:HA	1:Y:115:ILE:HD12	2.00	0.43
1:E:126:LEU:HG	3:E:2083:HOH:O	2.18	0.43
1:I:38:ALA:CB	1:I:43:ILE:HG13	2.48	0.43
1:K:53:GLU:HB2	3:L:2032:HOH:O	2.18	0.43
1:M:14:LEU:CD1	2:M:152:GOL:H11	2.28	0.43
1:R:18:GLU:HA	1:R:20:GLU:OE2	2.18	0.43
1:I:79:HIS:CE1	1:I:110:ARG:HA	2.53	0.43
1:V:25:GLN:HE21	1:V:30:ILE:HG12	1.82	0.43
1:B:81:SER:HB2	3:B:2046:HOH:O	2.17	0.43
2:K:152:GOL:H32	3:K:2082:HOH:O	2.19	0.43
1:M:2:HIS:HA	1:M:44:GLN:O	2.18	0.43
1:O:53:GLU:HB3	3:O:2035:HOH:O	2.19	0.43
1:X:53:GLU:HB2	3:Y:2025:HOH:O	2.17	0.43
1:H:100:LEU:HG	3:H:2066:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:PRO:CG	2:L:151:GOL:H12	2.43	0.43
1:M:123:ILE:HG22	3:M:2086:HOH:O	2.18	0.43
1:O:53:GLU:HB3	3:O:2034:HOH:O	2.18	0.43
1:R:17:ARG:O	1:R:18:GLU:C	2.61	0.43
1:S:24:ARG:HE	1:S:24:ARG:HB2	1.62	0.43
1:H:75:GLY:HA2	2:H:150:GOL:O2	2.19	0.43
1:P:113:SER:O	2:P:151:GOL:O1	2.32	0.43
2:R:151:GOL:H32	3:R:2099:HOH:O	2.18	0.43
1:S:79:HIS:CE1	3:S:2039:HOH:O	2.71	0.43
1:T:2:HIS:HA	1:T:44:GLN:O	2.19	0.43
1:C:22:PHE:CD2	2:C:152:GOL:H12	2.54	0.43
1:S:112:GLN:HB2	2:S:151:GOL:H31	2.00	0.43
1:Y:30:ILE:HG22	1:Y:34:LEU:HD12	2.00	0.43
1:R:40:ALA:O	1:R:42:HIS:N	2.48	0.43
1:Y:16:SER:O	1:Y:17:ARG:HB3	2.19	0.43
1:Y:43:ILE:CD1	1:Y:139:LEU:HD21	2.48	0.43
1:D:22:PHE:CE2	2:D:152:GOL:H32	2.54	0.43
1:J:122:GLN:HG2	1:J:124:VAL:HG23	2.01	0.43
1:P:136:ARG:O	1:P:139:LEU:HB2	2.19	0.43
1:S:79:HIS:CE1	1:S:110:ARG:HA	2.54	0.43
1:L:120:LYS:HA	1:L:120:LYS:HD3	1.90	0.42
1:N:82:TYR:HD1	3:N:2047:HOH:O	1.96	0.42
1:O:14:LEU:HD13	2:O:152:GOL:C1	2.49	0.42
1:R:113:SER:O	2:R:151:GOL:H12	2.18	0.42
1:H:99:HIS:CG	1:H:103:LEU:HD11	2.54	0.42
2:M:151:GOL:H2	1:P:111:HIS:ND1	2.33	0.42
2:S:150:GOL:C1	2:S:152:GOL:H31	2.47	0.42
1:T:103:LEU:HB2	3:T:2054:HOH:O	2.19	0.42
1:A:106:ARG:HH12	2:A:150:GOL:H12	1.84	0.42
1:B:6:LEU:HD22	1:B:56:LEU:HD22	2.02	0.42
1:R:141:GLN:HA	1:R:142:GLN:N	2.33	0.42
1:U:17:ARG:HG3	1:U:18:GLU:N	2.34	0.42
1:A:34:LEU:HA	1:A:37:PHE:HB3	2.01	0.42
1:D:30:ILE:HA	3:D:2021:HOH:O	2.19	0.42
1:I:112:GLN:HB2	2:I:151:GOL:H32	2.01	0.42
1:U:6:LEU:HD22	1:U:56:LEU:HD22	2.00	0.42
1:F:43:ILE:HG21	1:F:139:LEU:HD21	2.02	0.42
1:K:34:LEU:HD11	1:K:131:TYR:HB3	2.01	0.42
1:L:99:HIS:CG	1:L:103:LEU:HD11	2.54	0.42
1:M:7:ASN:O	1:M:49:GLN:HA	2.19	0.42
1:T:79:HIS:CE1	3:T:2039:HOH:O	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:81:SER:HB2	3:G:2046:HOH:O	2.19	0.42
1:N:116:ALA:N	1:N:117:PRO:CD	2.83	0.42
1:O:79:HIS:CE1	3:O:2055:HOH:O	2.71	0.42
1:U:78:SER:HA	1:U:115:ILE:HD12	2.01	0.42
2:R:152:GOL:H32	3:R:2006:HOH:O	2.19	0.42
1:J:80:TYR:HD1	3:J:2050:HOH:O	2.03	0.42
1:K:25:GLN:H	1:K:25:GLN:HG2	1.67	0.42
2:O:151:GOL:H2	1:V:111:HIS:ND1	2.35	0.42
1:A:22:PHE:CE2	2:A:152:GOL:H32	2.55	0.42
1:F:17:ARG:O	1:F:18:GLU:C	2.63	0.42
1:P:42:HIS:ND1	1:P:42:HIS:N	2.65	0.42
1:P:97:GLU:O	1:P:122:GLN:HA	2.20	0.42
1:R:103:LEU:HD12	3:R:2065:HOH:O	2.19	0.42
1:R:112:GLN:HB2	3:R:2099:HOH:O	2.18	0.42
1:U:2:HIS:NE2	1:U:46:THR:OG1	2.48	0.42
1:B:111:HIS:CG	2:G:151:GOL:H12	2.54	0.42
1:C:1:PRO:HG2	1:C:43:ILE:HG22	2.00	0.42
1:E:15:GLY:C	1:E:17:ARG:H	2.28	0.42
1:I:13:ARG:O	1:I:14:LEU:C	2.60	0.42
1:K:36:GLN:HB3	3:K:2018:HOH:O	2.20	0.42
1:P:1:PRO:CB	1:P:43:ILE:HG22	2.50	0.42
3:P:2033:HOH:O	1:R:77:LEU:CD2	2.67	0.42
1:V:103:LEU:HB2	3:V:2075:HOH:O	2.19	0.42
1:E:108:GLU:CD	3:E:2068:HOH:O	2.63	0.41
1:F:7:ASN:O	1:F:49:GLN:HA	2.19	0.41
1:L:15:GLY:O	1:L:16:SER:O	2.38	0.41
1:U:7:ASN:ND2	3:U:2001:HOH:O	2.52	0.41
1:V:66:GLN:HG3	3:V:2052:HOH:O	2.19	0.41
1:J:78:SER:HA	1:J:115:ILE:HD12	2.01	0.41
1:S:22:PHE:CE2	2:S:152:GOL:H11	2.55	0.41
1:C:22:PHE:CE2	2:C:152:GOL:H12	2.55	0.41
1:G:112[B]:GLN:CG	2:G:151:GOL:H2	2.35	0.41
1:K:113:SER:O	2:K:151:GOL:O1	2.37	0.41
1:M:6:LEU:HD13	1:M:72:LEU:HD13	2.01	0.41
1:R:79:HIS:CE1	1:R:110:ARG:HA	2.55	0.41
1:R:128:ALA:HA	3:R:2087:HOH:O	2.19	0.41
1:S:43:ILE:HD13	1:S:139:LEU:HD21	2.01	0.41
1:U:43:ILE:HD13	1:U:139:LEU:HD11	2.02	0.41
1:G:6:LEU:HD22	1:G:56:LEU:HD22	2.03	0.41
1:R:99:HIS:CG	1:R:103:LEU:HD11	2.55	0.41
1:M:99:HIS:CG	1:M:103:LEU:HD11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:103:LEU:HB2	3:Q:2073:HOH:O	2.20	0.41
1:G:23:GLY:O	1:G:24:ARG:CB	2.68	0.41
1:S:25:GLN:HB3	1:S:29:ASP:CB	2.50	0.41
1:Y:103:LEU:CD1	3:Y:2059:HOH:O	2.58	0.41
1:E:80:TYR:HE1	3:F:2034:HOH:O	2.02	0.41
1:I:31:GLU:HG3	1:I:47:PHE:CE1	2.55	0.41
1:M:120:LYS:NZ	3:M:2082:HOH:O	2.53	0.41
3:M:2021:HOH:O	1:O:80:TYR:HD1	2.04	0.41
1:T:124:VAL:HG21	3:T:2054:HOH:O	2.21	0.41
1:G:35:PHE:O	1:G:38:ALA:HB3	2.21	0.41
1:P:6:LEU:HD22	1:P:56:LEU:HD22	2.03	0.41
1:U:18:GLU:O	1:U:22:PHE:HB2	2.21	0.41
1:C:2:HIS:NE2	1:C:46:THR:OG1	2.49	0.41
1:C:116:ALA:N	1:C:117:PRO:CD	2.84	0.41
1:E:41:LEU:O	1:E:42:HIS:C	2.62	0.41
1:G:13:ARG:HD3	1:H:61:HIS:CG	2.56	0.41
1:H:27:LEU:HD11	3:H:2070:HOH:O	2.21	0.41
1:L:43:ILE:CG2	1:L:139:LEU:HD21	2.51	0.41
1:S:19:PRO:HA	1:S:23:GLY:N	2.36	0.41
1:S:53:GLU:OE2	1:S:81:SER:OG	2.33	0.41
1:T:14:LEU:HD13	2:T:152:GOL:H11	2.03	0.41
1:E:1:PRO:H2	1:E:43:ILE:HG22	1.86	0.41
1:I:108:GLU:HG2	3:I:2062:HOH:O	2.21	0.41
1:J:43:ILE:HG21	1:J:139:LEU:HD11	2.03	0.41
1:J:79:HIS:CE1	1:J:110:ARG:HA	2.56	0.41
1:L:7:ASN:O	1:L:49:GLN:HA	2.21	0.41
1:B:112:GLN:HG3	2:B:151:GOL:H31	2.02	0.40
1:E:81:SER:HB2	3:E:2034:HOH:O	2.21	0.40
1:F:25:GLN:HE21	1:F:25:GLN:HB3	1.71	0.40
1:H:40:ALA:O	1:H:41:LEU:CB	2.69	0.40
1:J:99:HIS:CG	1:J:103:LEU:HD11	2.55	0.40
1:M:18:GLU:HA	1:M:19:PRO:HD3	1.93	0.40
1:O:2:HIS:HA	1:O:44:GLN:O	2.21	0.40
1:U:1:PRO:HD2	1:U:43:ILE:HG22	2.03	0.40
1:U:14:LEU:HA	2:U:152:GOL:H11	2.04	0.40
1:E:30:ILE:O	1:E:34:LEU:HG	2.21	0.40
1:L:17:ARG:NH1	3:L:2009:HOH:O	2.53	0.40
1:Q:12:ASN:HA	1:Q:27:LEU:CD2	2.52	0.40
1:Q:12:ASN:HA	1:Q:27:LEU:HD23	2.03	0.40
1:A:18:GLU:OE1	1:A:21:VAL:HG21	2.22	0.40
1:I:138:LEU:O	1:I:141:GLN:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:10:ASN:HB2	3:L:2003:HOH:O	2.20	0.40
1:S:112:GLN:CG	2:S:151:GOL:H31	2.52	0.40
1:V:79:HIS:CE1	3:V:2058:HOH:O	2.74	0.40
1:Y:79:HIS:CE1	3:Y:2034:HOH:O	2.74	0.40
1:H:43:ILE:CD1	1:H:139:LEU:HD11	2.51	0.40
1:H:99:HIS:CE1	3:H:2038:HOH:O	2.74	0.40
1:I:141:GLN:HE21	1:I:142:GLN:N	2.14	0.40
1:K:10:ASN:O	2:K:152:GOL:O2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
1	B	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	18	15
1	C	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	D	140/143 (98%)	132 (94%)	7 (5%)	1 (1%)	18	15
1	E	142/143 (99%)	130 (92%)	10 (7%)	2 (1%)	9	5
1	F	142/143 (99%)	133 (94%)	7 (5%)	2 (1%)	9	5
1	G	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	9	5
1	H	140/143 (98%)	132 (94%)	8 (6%)	0	100	100
1	I	139/143 (97%)	130 (94%)	5 (4%)	4 (3%)	3	1
1	J	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	K	132/143 (92%)	127 (96%)	5 (4%)	0	100	100
1	L	140/143 (98%)	128 (91%)	6 (4%)	6 (4%)	2	0
1	M	140/143 (98%)	133 (95%)	5 (4%)	2 (1%)	9	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	128/143 (90%)	124 (97%)	4 (3%)	0	100	100
1	O	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	P	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	9	5
1	Q	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	R	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	18	15
1	S	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	T	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	18	15
1	U	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	9	5
1	V	131/143 (92%)	125 (95%)	5 (4%)	1 (1%)	16	12
1	X	129/143 (90%)	122 (95%)	7 (5%)	0	100	100
1	Y	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	18	15
All	All	3314/3432 (97%)	3130 (94%)	156 (5%)	28 (1%)	16	12

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	16	SER
1	L	22	PHE
1	L	23	GLY
1	P	16	SER
1	V	16	SER
1	E	16[A]	SER
1	E	16[B]	SER
1	G	24	ARG
1	I	14	LEU
1	I	25	GLN
1	L	16	SER
1	L	20	GLU
1	L	24	ARG
1	M	22	PHE
1	P	25	GLN
1	F	25	GLN
1	U	16	SER
1	F	18	GLU
1	I	18	GLU
1	R	26	THR
1	B	18	GLU
1	T	18	GLU

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Mol	Chain	Res	Type
1	U	18	GLU
1	Y	18	GLU
1	D	18	GLU
1	G	18	GLU
1	M	21	VAL
1	L	19	PRO

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	115/120 (96%)	105 (91%)	10 (9%)	9	7
1	B	115/120 (96%)	105 (91%)	10 (9%)	9	7
1	C	115/120 (96%)	109 (95%)	6 (5%)	21	20
1	D	115/120 (96%)	102 (89%)	13 (11%)	5	3
1	E	119/120 (99%)	110 (92%)	9 (8%)	12	9
1	F	119/120 (99%)	110 (92%)	9 (8%)	12	9
1	G	117/120 (98%)	105 (90%)	12 (10%)	7	4
1	H	115/120 (96%)	102 (89%)	13 (11%)	5	3
1	I	114/120 (95%)	103 (90%)	11 (10%)	8	5
1	J	115/120 (96%)	108 (94%)	7 (6%)	17	15
1	K	110/120 (92%)	100 (91%)	10 (9%)	9	6
1	L	113/120 (94%)	103 (91%)	10 (9%)	9	7
1	M	116/120 (97%)	107 (92%)	9 (8%)	11	9
1	N	109/120 (91%)	102 (94%)	7 (6%)	16	14
1	O	115/120 (96%)	108 (94%)	7 (6%)	17	15
1	P	116/120 (97%)	105 (90%)	11 (10%)	8	5
1	Q	118/120 (98%)	109 (92%)	9 (8%)	12	9
1	R	115/120 (96%)	106 (92%)	9 (8%)	11	9
1	S	118/120 (98%)	106 (90%)	12 (10%)	7	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	118/120 (98%)	107 (91%)	11 (9%)	8	6
1	U	115/120 (96%)	105 (91%)	10 (9%)	9	7
1	V	112/120 (93%)	104 (93%)	8 (7%)	13	11
1	X	110/120 (92%)	103 (94%)	7 (6%)	16	14
1	Y	115/120 (96%)	100 (87%)	15 (13%)	4	2
All	All	2759/2880 (96%)	2524 (92%)	235 (8%)	10	7

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	LEU
1	A	14	LEU
1	A	16	SER
1	A	22	PHE
1	A	28	THR
1	A	33	ASP
1	A	42	HIS
1	A	112	GLN
1	A	138	LEU
1	B	1	PRO
1	B	4	LEU
1	B	6	LEU
1	B	14	LEU
1	B	16	SER
1	B	20	GLU
1	B	25	GLN
1	B	33	ASP
1	B	112	GLN
1	B	138	LEU
1	C	4	LEU
1	C	6	LEU
1	C	14	LEU
1	C	20	GLU
1	C	112	GLN
1	C	138	LEU
1	D	4	LEU
1	D	6	LEU
1	D	14	LEU
1	D	17	ARG

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Mol	Chain	Res	Type
1	D	20	GLU
1	D	21	VAL
1	D	22	PHE
1	D	25	GLN
1	D	64	GLU
1	D	74	PRO
1	D	112[A]	GLN
1	D	112[B]	GLN
1	D	138	LEU
1	E	4	LEU
1	E	6	LEU
1	E	14	LEU
1	E	25	GLN
1	E	33	ASP
1	E	41	LEU
1	E	43	ILE
1	E	112	GLN
1	E	138	LEU
1	F	4	LEU
1	F	6	LEU
1	F	14	LEU
1	F	20	GLU
1	F	25	GLN
1	F	68	SER
1	F	112[A]	GLN
1	F	112[B]	GLN
1	F	138	LEU
1	G	4	LEU
1	G	6	LEU
1	G	14	LEU
1	G	16[A]	SER
1	G	16[B]	SER
1	G	20	GLU
1	G	43	ILE
1	G	64	GLU
1	G	112[A]	GLN
1	G	112[B]	GLN
1	G	138	LEU
1	G	139	LEU
1	H	4	LEU
1	H	6	LEU
1	H	14	LEU

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Mol	Chain	Res	Type
1	H	20	GLU
1	H	25	GLN
1	H	33	ASP
1	H	37	PHE
1	H	42	HIS
1	H	43	ILE
1	H	64	GLU
1	H	112	GLN
1	H	138	LEU
1	H	140	SER
1	I	4	LEU
1	I	6	LEU
1	I	14	LEU
1	I	25	GLN
1	I	33	ASP
1	I	34	LEU
1	I	37	PHE
1	I	64	GLU
1	I	112	GLN
1	I	138	LEU
1	I	140	SER
1	J	4	LEU
1	J	6	LEU
1	J	14	LEU
1	J	25	GLN
1	J	41	LEU
1	J	112	GLN
1	J	138	LEU
1	K	1	PRO
1	K	4	LEU
1	K	6	LEU
1	K	14	LEU
1	K	17	ARG
1	K	25	GLN
1	K	42	HIS
1	K	64	GLU
1	K	112	GLN
1	K	138	LEU
1	L	4	LEU
1	L	6	LEU
1	L	14	LEU
1	L	16	SER

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Mol	Chain	Res	Type
1	L	25	GLN
1	L	36	GLN
1	L	112[A]	GLN
1	L	112[B]	GLN
1	L	138	LEU
1	L	140	SER
1	M	4	LEU
1	M	6	LEU
1	M	14	LEU
1	M	17	ARG
1	M	31	GLU
1	M	41	LEU
1	M	112	GLN
1	M	138	LEU
1	M	140	SER
1	N	4	LEU
1	N	6	LEU
1	N	14	LEU
1	N	25	GLN
1	N	112	GLN
1	N	138	LEU
1	N	140	SER
1	O	4	LEU
1	O	6	LEU
1	O	14	LEU
1	O	24	ARG
1	O	64	GLU
1	O	112	GLN
1	O	138	LEU
1	P	4	LEU
1	P	6	LEU
1	P	14	LEU
1	P	16	SER
1	P	17	ARG
1	P	20	GLU
1	P	43	ILE
1	P	64	GLU
1	P	112	GLN
1	P	138	LEU
1	P	140	SER
1	Q	4	LEU
1	Q	6	LEU

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Mol	Chain	Res	Type
1	Q	14	LEU
1	Q	35	PHE
1	Q	64	GLU
1	Q	74	PRO
1	Q	112	GLN
1	Q	138	LEU
1	Q	139	LEU
1	R	1	PRO
1	R	4	LEU
1	R	6	LEU
1	R	14	LEU
1	R	20	GLU
1	R	25	GLN
1	R	64	GLU
1	R	112	GLN
1	R	138	LEU
1	S	1	PRO
1	S	4	LEU
1	S	6	LEU
1	S	14	LEU
1	S	17	ARG
1	S	19	PRO
1	S	20	GLU
1	S	24	ARG
1	S	25	GLN
1	S	64	GLU
1	S	112	GLN
1	S	138	LEU
1	T	4	LEU
1	T	6	LEU
1	T	14	LEU
1	T	18	GLU
1	T	20	GLU
1	T	28	THR
1	T	35	PHE
1	T	43	ILE
1	T	112	GLN
1	T	138	LEU
1	T	139	LEU
1	U	4	LEU
1	U	6	LEU
1	U	14	LEU

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Mol	Chain	Res	Type
1	U	17	ARG
1	U	20	GLU
1	U	41	LEU
1	U	68	SER
1	U	112	GLN
1	U	138	LEU
1	U	139	LEU
1	V	4	LEU
1	V	6	LEU
1	V	14	LEU
1	V	25	GLN
1	V	35	PHE
1	V	68	SER
1	V	112	GLN
1	V	138	LEU
1	X	4	LEU
1	X	6	LEU
1	X	14	LEU
1	X	16	SER
1	X	68	SER
1	X	112	GLN
1	X	138	LEU
1	Y	1	PRO
1	Y	4	LEU
1	Y	6	LEU
1	Y	14	LEU
1	Y	20	GLU
1	Y	25	GLN
1	Y	34	LEU
1	Y	35	PHE
1	Y	37	PHE
1	Y	42	HIS
1	Y	43	ILE
1	Y	74	PRO
1	Y	112	GLN
1	Y	138	LEU
1	Y	140	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN

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Mol	Chain	Res	Type
1	A	122	GLN
1	A	141	GLN
1	B	25	GLN
1	B	122	GLN
1	C	122	GLN
1	D	25	GLN
1	D	66	GLN
1	D	122	GLN
1	E	122	GLN
1	F	25	GLN
1	F	122	GLN
1	G	25	GLN
1	G	66	GLN
1	H	122	GLN
1	H	141	GLN
1	I	25	GLN
1	I	36	GLN
1	I	42	HIS
1	I	66	GLN
1	J	141	GLN
1	L	66	GLN
1	L	122	GLN
1	L	141	GLN
1	M	66	GLN
1	M	122	GLN
1	N	36	GLN
1	O	122	GLN
1	P	36	GLN
1	P	66	GLN
1	Q	36	GLN
1	Q	66	GLN
1	Q	122	GLN
1	R	36	GLN
1	R	66	GLN
1	S	25	GLN
1	S	112	GLN
1	S	122	GLN
1	U	66	GLN
1	U	122	GLN
1	V	25	GLN
1	V	66	GLN
1	X	36	GLN

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Mol	Chain	Res	Type
1	X	122	GLN
1	Y	25	GLN
1	Y	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

72 ligands are modelled in this entry.

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	$\# Z > 2$
2	GOL	A	151	-	5,5,5	0.70	0	5,5,5	2.11	2 (40%)
2	GOL	A	152	-	5,5,5	0.77	0	5,5,5	1.03	0
2	GOL	B	151	-	5,5,5	0.90	0	5,5,5	1.26	1 (20%)
2	GOL	X	151	-	5,5,5	0.79	0	5,5,5	1.72	1 (20%)
2	GOL	K	150	-	5,5,5	1.11	1 (20%)	5,5,5	1.25	0
2	GOL	K	151	-	5,5,5	0.70	0	5,5,5	0.62	0
2	GOL	B	152	-	5,5,5	0.68	0	5,5,5	0.48	0
2	GOL	I	150	-	5,5,5	0.79	0	5,5,5	1.75	3 (60%)
2	GOL	A	150	-	5,5,5	0.97	0	5,5,5	0.52	0
2	GOL	K	152	-	5,5,5	0.82	0	5,5,5	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	N	150	-	5,5,5	1.20	0	5,5,5	1.58	1 (20%)
2	GOL	I	152	-	5,5,5	0.57	0	5,5,5	1.04	0
2	GOL	N	151	-	5,5,5	0.75	0	5,5,5	1.55	1 (20%)
2	GOL	S	151	-	5,5,5	0.80	0	5,5,5	1.80	2 (40%)
2	GOL	T	151	-	5,5,5	0.67	0	5,5,5	0.55	0
2	GOL	N	152	-	5,5,5	0.69	0	5,5,5	0.91	0
2	GOL	Q	151	-	5,5,5	0.78	0	5,5,5	0.52	0
2	GOL	S	150	-	5,5,5	1.86	1 (20%)	5,5,5	1.48	1 (20%)
2	GOL	X	152	-	5,5,5	0.85	0	5,5,5	0.46	0
2	GOL	P	151	-	5,5,5	0.79	0	5,5,5	0.83	0
2	GOL	U	151	-	5,5,5	0.43	0	5,5,5	0.80	0
2	GOL	I	151	-	5,5,5	0.63	0	5,5,5	0.93	0
2	GOL	F	150	-	5,5,5	1.18	0	5,5,5	1.88	3 (60%)
2	GOL	F	151	-	5,5,5	0.60	0	5,5,5	0.82	0
2	GOL	S	152	-	5,5,5	0.62	0	5,5,5	1.00	0
2	GOL	U	152	-	5,5,5	0.79	0	5,5,5	0.70	0
2	GOL	F	152	-	4,4,5	1.13	0	4,4,5	0.75	0
2	GOL	Y	151	-	5,5,5	0.56	0	5,5,5	0.94	0
2	GOL	E	150	-	5,5,5	1.11	1 (20%)	5,5,5	0.93	0
2	GOL	E	151	-	5,5,5	0.63	0	5,5,5	0.84	0
2	GOL	H	150	-	5,5,5	0.96	0	5,5,5	1.50	1 (20%)
2	GOL	U	150	-	5,5,5	0.99	0	5,5,5	1.53	1 (20%)
2	GOL	C	151	-	5,5,5	0.82	0	5,5,5	1.04	0
2	GOL	J	150	-	5,5,5	0.95	0	5,5,5	2.40	2 (40%)
2	GOL	J	151	-	5,5,5	0.71	0	5,5,5	1.32	1 (20%)
2	GOL	O	150	-	5,5,5	1.30	1 (20%)	5,5,5	1.78	1 (20%)
2	GOL	O	151	-	5,5,5	0.85	0	5,5,5	1.13	1 (20%)
2	GOL	L	150	-	5,5,5	0.98	1 (20%)	5,5,5	2.33	2 (40%)
2	GOL	P	150	-	5,5,5	1.18	1 (20%)	5,5,5	1.18	0
2	GOL	O	152	-	5,5,5	0.79	0	5,5,5	0.57	0
2	GOL	B	150	-	5,5,5	0.84	0	5,5,5	1.21	0
2	GOL	E	152	-	4,4,5	0.95	0	4,4,5	0.77	0
2	GOL	T	152	-	5,5,5	0.72	0	5,5,5	0.75	0
2	GOL	M	150	-	5,5,5	1.11	0	5,5,5	1.25	0
2	GOL	J	152	-	5,5,5	0.83	0	5,5,5	1.14	1 (20%)
2	GOL	M	152	-	5,5,5	0.54	0	5,5,5	0.99	0
2	GOL	C	150	-	5,5,5	1.12	0	5,5,5	1.29	1 (20%)
2	GOL	X	150	-	5,5,5	1.40	1 (20%)	5,5,5	1.08	0
2	GOL	C	152	-	5,5,5	0.83	0	5,5,5	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	D	151	-	5,5,5	0.90	0	5,5,5	0.74	0
2	GOL	Q	150	-	5,5,5	1.15	0	5,5,5	1.51	1 (20%)
2	GOL	T	150	-	5,5,5	1.07	0	5,5,5	1.70	1 (20%)
2	GOL	V	150	-	5,5,5	0.61	0	5,5,5	1.14	1 (20%)
2	GOL	G	151	-	5,5,5	0.65	0	5,5,5	1.47	1 (20%)
2	GOL	Q	152	-	5,5,5	0.96	0	5,5,5	0.77	0
2	GOL	R	152	-	5,5,5	0.68	0	5,5,5	0.80	0
2	GOL	Y	152	-	5,5,5	1.00	0	5,5,5	0.76	0
2	GOL	D	150	-	5,5,5	1.05	0	5,5,5	2.34	2 (40%)
2	GOL	Y	150	-	5,5,5	0.71	0	5,5,5	1.68	2 (40%)
2	GOL	H	151	-	5,5,5	0.77	0	5,5,5	0.80	0
2	GOL	G	150	-	5,5,5	0.59	0	5,5,5	1.19	1 (20%)
2	GOL	D	152	-	5,5,5	0.52	0	5,5,5	2.02	4 (80%)
2	GOL	M	151	-	5,5,5	0.63	0	5,5,5	0.94	0
2	GOL	R	150	-	5,5,5	1.89	2 (40%)	5,5,5	2.39	3 (60%)
2	GOL	R	151	-	5,5,5	0.47	0	5,5,5	1.53	2 (40%)
2	GOL	L	151	-	5,5,5	0.58	0	5,5,5	0.86	0
2	GOL	V	151	-	5,5,5	0.73	0	5,5,5	2.00	1 (20%)
2	GOL	H	152	-	5,5,5	0.83	0	5,5,5	1.20	0
2	GOL	L	152	-	5,5,5	0.56	0	5,5,5	1.16	0
2	GOL	G	152	-	5,5,5	0.72	0	5,5,5	1.94	2 (40%)
2	GOL	P	152	-	5,5,5	0.71	0	5,5,5	0.72	0
2	GOL	V	152	-	5,5,5	0.74	0	5,5,5	1.33	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
2	GOL	A	151	-	-	3/4/4/4	-
2	GOL	A	152	-	-	4/4/4/4	-
2	GOL	B	151	-	-	2/4/4/4	-
2	GOL	X	151	-	-	1/4/4/4	-
2	GOL	K	150	-	-	1/4/4/4	-
2	GOL	K	151	-	-	2/4/4/4	-
2	GOL	B	152	-	-	4/4/4/4	-
2	GOL	I	150	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	150	-	-	2/4/4/4	-
2	GOL	K	152	-	-	1/4/4/4	-
2	GOL	N	150	-	-	2/4/4/4	-
2	GOL	I	152	-	-	2/4/4/4	-
2	GOL	N	151	-	-	4/4/4/4	-
2	GOL	S	151	-	-	2/4/4/4	-
2	GOL	T	151	-	-	2/4/4/4	-
2	GOL	N	152	-	-	4/4/4/4	-
2	GOL	Q	151	-	-	4/4/4/4	-
2	GOL	S	150	-	-	4/4/4/4	-
2	GOL	X	152	-	-	2/4/4/4	-
2	GOL	P	151	-	-	4/4/4/4	-
2	GOL	U	151	-	-	4/4/4/4	-
2	GOL	I	151	-	-	3/4/4/4	-
2	GOL	F	150	-	-	3/4/4/4	-
2	GOL	F	151	-	-	3/4/4/4	-
2	GOL	S	152	-	-	2/4/4/4	-
2	GOL	U	152	-	-	2/4/4/4	-
2	GOL	F	152	-	-	2/2/2/4	-
2	GOL	Y	151	-	-	2/4/4/4	-
2	GOL	E	150	-	-	1/4/4/4	-
2	GOL	E	151	-	-	4/4/4/4	-
2	GOL	H	150	-	-	2/4/4/4	-
2	GOL	U	150	-	-	4/4/4/4	-
2	GOL	C	151	-	-	2/4/4/4	-
2	GOL	J	150	-	-	2/4/4/4	-
2	GOL	J	151	-	-	2/4/4/4	-
2	GOL	O	150	-	-	4/4/4/4	-
2	GOL	O	151	-	-	2/4/4/4	-
2	GOL	L	150	-	-	3/4/4/4	-
2	GOL	P	150	-	-	3/4/4/4	-
2	GOL	O	152	-	-	2/4/4/4	-
2	GOL	B	150	-	-	2/4/4/4	-
2	GOL	E	152	-	-	0/2/2/4	-
2	GOL	T	152	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	M	150	-	-	4/4/4/4	-
2	GOL	J	152	-	-	2/4/4/4	-
2	GOL	M	152	-	-	3/4/4/4	-
2	GOL	C	150	-	-	2/4/4/4	-
2	GOL	X	150	-	-	4/4/4/4	-
2	GOL	C	152	-	-	0/4/4/4	-
2	GOL	D	151	-	-	4/4/4/4	-
2	GOL	Q	150	-	-	2/4/4/4	-
2	GOL	T	150	-	-	2/4/4/4	-
2	GOL	V	150	-	-	3/4/4/4	-
2	GOL	G	151	-	-	1/4/4/4	-
2	GOL	Q	152	-	-	2/4/4/4	-
2	GOL	R	152	-	-	1/4/4/4	-
2	GOL	Y	152	-	-	1/4/4/4	-
2	GOL	D	150	-	-	2/4/4/4	-
2	GOL	Y	150	-	-	1/4/4/4	-
2	GOL	H	151	-	-	2/4/4/4	-
2	GOL	G	150	-	-	0/4/4/4	-
2	GOL	D	152	-	-	3/4/4/4	-
2	GOL	M	151	-	-	3/4/4/4	-
2	GOL	R	150	-	-	2/4/4/4	-
2	GOL	R	151	-	-	1/4/4/4	-
2	GOL	L	151	-	-	2/4/4/4	-
2	GOL	V	151	-	-	3/4/4/4	-
2	GOL	H	152	-	-	2/4/4/4	-
2	GOL	L	152	-	-	2/4/4/4	-
2	GOL	G	152	-	-	3/4/4/4	-
2	GOL	P	152	-	-	4/4/4/4	-
2	GOL	V	152	-	-	4/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	150	GOL	O1-C1	3.67	1.57	1.42
2	R	150	GOL	C1-C2	2.77	1.62	1.51
2	X	150	GOL	O1-C1	2.71	1.53	1.42
2	E	150	GOL	C1-C2	2.16	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	150	GOL	C1-C2	2.15	1.60	1.51
2	K	150	GOL	O1-C1	2.12	1.51	1.42
2	R	150	GOL	O1-C1	2.11	1.51	1.42
2	P	150	GOL	O1-C1	2.09	1.51	1.42
2	L	150	GOL	O1-C1	2.02	1.50	1.42

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	150	GOL	C3-C2-C1	4.32	127.66	111.80
2	V	151	GOL	O2-C2-C1	3.99	125.71	109.18
2	L	150	GOL	C3-C2-C1	3.85	125.92	111.80
2	D	150	GOL	O1-C1-C2	-3.62	94.07	110.38
2	A	151	GOL	O2-C2-C1	3.50	123.68	109.18
2	T	150	GOL	O3-C3-C2	3.43	125.83	110.38
2	X	151	GOL	C3-C2-C1	3.24	123.67	111.80
2	R	150	GOL	O1-C1-C2	-3.19	96.00	110.38
2	G	151	GOL	O2-C2-C1	3.12	122.08	109.18
2	G	152	GOL	O2-C2-C1	3.11	122.06	109.18
2	L	150	GOL	O3-C3-C2	3.06	124.17	110.38
2	H	150	GOL	O3-C3-C2	3.01	123.92	110.38
2	D	150	GOL	O2-C2-C3	2.96	121.45	109.18
2	Y	150	GOL	O3-C3-C2	2.92	123.50	110.38
2	S	151	GOL	O2-C2-C1	2.89	121.14	109.18
2	N	151	GOL	O2-C2-C1	2.86	121.01	109.18
2	Q	150	GOL	O1-C1-C2	-2.80	97.78	110.38
2	R	150	GOL	C3-C2-C1	-2.79	101.55	111.80
2	U	150	GOL	O1-C1-C2	-2.76	97.94	110.38
2	J	150	GOL	O3-C3-C2	2.75	122.77	110.38
2	J	151	GOL	O2-C2-C1	2.75	120.57	109.18
2	C	150	GOL	O2-C2-C3	-2.75	97.81	109.18
2	F	150	GOL	C3-C2-C1	2.72	121.76	111.80
2	G	152	GOL	O2-C2-C3	2.65	120.17	109.18
2	S	151	GOL	O2-C2-C3	2.62	120.04	109.18
2	N	150	GOL	O1-C1-C2	-2.60	98.69	110.38
2	O	150	GOL	O3-C3-C2	2.59	122.03	110.38
2	R	150	GOL	O3-C3-C2	2.57	121.94	110.38
2	D	152	GOL	O2-C2-C1	2.50	119.53	109.18
2	A	151	GOL	O1-C1-C2	2.50	121.62	110.38
2	S	150	GOL	O1-C1-C2	-2.47	99.24	110.38
2	I	150	GOL	O1-C1-C2	-2.37	99.72	110.38
2	J	152	GOL	O3-C3-C2	2.36	121.00	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	150	GOL	O2-C2-C1	2.35	118.91	109.18
2	D	152	GOL	O3-C3-C2	2.29	120.67	110.38
2	Y	150	GOL	O2-C2-C1	2.20	118.30	109.18
2	R	151	GOL	O1-C1-C2	2.20	120.28	110.38
2	G	150	GOL	O2-C2-C1	2.20	118.27	109.18
2	D	152	GOL	O2-C2-C3	2.18	118.20	109.18
2	B	151	GOL	O1-C1-C2	2.06	119.65	110.38
2	I	150	GOL	C3-C2-C1	2.06	119.33	111.80
2	D	152	GOL	C3-C2-C1	2.04	119.27	111.80
2	I	150	GOL	O2-C2-C3	2.02	117.53	109.18
2	F	150	GOL	O1-C1-C2	-2.02	101.30	110.38
2	R	151	GOL	O3-C3-C2	2.01	119.44	110.38
2	V	150	GOL	O2-C2-C1	2.01	117.50	109.18
2	O	151	GOL	O2-C2-C1	2.01	117.49	109.18

There are no chirality outliers.

All (174) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	150	GOL	C1-C2-C3-O3
2	A	151	GOL	O1-C1-C2-C3
2	A	152	GOL	C1-C2-C3-O3
2	B	150	GOL	O1-C1-C2-C3
2	B	152	GOL	C1-C2-C3-O3
2	B	152	GOL	O2-C2-C3-O3
2	C	151	GOL	O1-C1-C2-O2
2	D	150	GOL	O1-C1-C2-C3
2	D	151	GOL	C1-C2-C3-O3
2	D	152	GOL	O1-C1-C2-O2
2	D	152	GOL	O2-C2-C3-O3
2	E	151	GOL	O1-C1-C2-C3
2	E	151	GOL	C1-C2-C3-O3
2	E	151	GOL	O2-C2-C3-O3
2	F	150	GOL	O1-C1-C2-C3
2	F	151	GOL	O1-C1-C2-C3
2	F	152	GOL	O1-C1-C2-O2
2	F	152	GOL	O1-C1-C2-C3
2	G	152	GOL	C1-C2-C3-O3
2	H	150	GOL	O1-C1-C2-C3
2	H	152	GOL	O1-C1-C2-C3
2	I	150	GOL	O1-C1-C2-C3
2	I	151	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	K	150	GOL	O1-C1-C2-C3
2	L	150	GOL	O2-C2-C3-O3
2	M	150	GOL	O1-C1-C2-C3
2	M	150	GOL	C1-C2-C3-O3
2	M	151	GOL	O1-C1-C2-C3
2	M	151	GOL	C1-C2-C3-O3
2	N	150	GOL	O1-C1-C2-C3
2	N	151	GOL	O1-C1-C2-C3
2	N	151	GOL	C1-C2-C3-O3
2	N	152	GOL	O1-C1-C2-O2
2	N	152	GOL	O1-C1-C2-C3
2	N	152	GOL	C1-C2-C3-O3
2	O	150	GOL	O1-C1-C2-C3
2	P	150	GOL	O1-C1-C2-C3
2	P	151	GOL	O1-C1-C2-C3
2	P	151	GOL	C1-C2-C3-O3
2	P	151	GOL	O2-C2-C3-O3
2	P	152	GOL	C1-C2-C3-O3
2	Q	150	GOL	O1-C1-C2-C3
2	Q	151	GOL	O1-C1-C2-O2
2	Q	151	GOL	C1-C2-C3-O3
2	R	150	GOL	O1-C1-C2-C3
2	S	150	GOL	O1-C1-C2-C3
2	S	151	GOL	C1-C2-C3-O3
2	T	150	GOL	O1-C1-C2-C3
2	T	151	GOL	O1-C1-C2-C3
2	T	152	GOL	C1-C2-C3-O3
2	U	150	GOL	O1-C1-C2-C3
2	U	151	GOL	C1-C2-C3-O3
2	U	152	GOL	C1-C2-C3-O3
2	U	152	GOL	O2-C2-C3-O3
2	V	150	GOL	O1-C1-C2-C3
2	V	151	GOL	O1-C1-C2-C3
2	V	152	GOL	C1-C2-C3-O3
2	X	150	GOL	C1-C2-C3-O3
2	A	150	GOL	O2-C2-C3-O3
2	A	151	GOL	O1-C1-C2-O2
2	F	151	GOL	O1-C1-C2-O2
2	J	152	GOL	O2-C2-C3-O3
2	M	151	GOL	O1-C1-C2-O2
2	N	151	GOL	O1-C1-C2-O2
2	N	152	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	S	150	GOL	O2-C2-C3-O3
2	S	151	GOL	O1-C1-C2-O2
2	A	151	GOL	C1-C2-C3-O3
2	A	152	GOL	O1-C1-C2-C3
2	B	151	GOL	C1-C2-C3-O3
2	C	150	GOL	C1-C2-C3-O3
2	C	151	GOL	O1-C1-C2-C3
2	D	151	GOL	O1-C1-C2-C3
2	D	152	GOL	O1-C1-C2-C3
2	E	150	GOL	C1-C2-C3-O3
2	F	151	GOL	C1-C2-C3-O3
2	G	151	GOL	O1-C1-C2-C3
2	H	151	GOL	C1-C2-C3-O3
2	I	150	GOL	C1-C2-C3-O3
2	I	151	GOL	O1-C1-C2-C3
2	J	150	GOL	O1-C1-C2-C3
2	J	151	GOL	O1-C1-C2-C3
2	J	152	GOL	C1-C2-C3-O3
2	K	151	GOL	C1-C2-C3-O3
2	L	150	GOL	O1-C1-C2-C3
2	L	151	GOL	O1-C1-C2-C3
2	M	152	GOL	O1-C1-C2-C3
2	M	152	GOL	C1-C2-C3-O3
2	O	150	GOL	C1-C2-C3-O3
2	O	151	GOL	C1-C2-C3-O3
2	O	152	GOL	O1-C1-C2-C3
2	P	150	GOL	C1-C2-C3-O3
2	P	152	GOL	O1-C1-C2-C3
2	Q	151	GOL	O1-C1-C2-C3
2	Q	152	GOL	O1-C1-C2-C3
2	R	151	GOL	C1-C2-C3-O3
2	S	150	GOL	C1-C2-C3-O3
2	S	152	GOL	C1-C2-C3-O3
2	U	150	GOL	C1-C2-C3-O3
2	U	151	GOL	O1-C1-C2-C3
2	V	152	GOL	O1-C1-C2-C3
2	X	150	GOL	O1-C1-C2-C3
2	X	152	GOL	C1-C2-C3-O3
2	Y	151	GOL	O1-C1-C2-C3
2	Y	152	GOL	O1-C1-C2-C3
2	B	150	GOL	O1-C1-C2-O2
2	F	150	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	H	150	GOL	O1-C1-C2-O2
2	I	150	GOL	O2-C2-C3-O3
2	I	151	GOL	O2-C2-C3-O3
2	J	150	GOL	O1-C1-C2-O2
2	L	152	GOL	O2-C2-C3-O3
2	M	150	GOL	O2-C2-C3-O3
2	M	152	GOL	O2-C2-C3-O3
2	N	150	GOL	O1-C1-C2-O2
2	O	150	GOL	O1-C1-C2-O2
2	O	151	GOL	O2-C2-C3-O3
2	P	151	GOL	O1-C1-C2-O2
2	Q	150	GOL	O1-C1-C2-O2
2	Q	152	GOL	O1-C1-C2-O2
2	R	150	GOL	O1-C1-C2-O2
2	S	150	GOL	O1-C1-C2-O2
2	S	152	GOL	O2-C2-C3-O3
2	T	150	GOL	O1-C1-C2-O2
2	T	151	GOL	O1-C1-C2-O2
2	T	152	GOL	O2-C2-C3-O3
2	U	150	GOL	O2-C2-C3-O3
2	U	151	GOL	O2-C2-C3-O3
2	V	150	GOL	O1-C1-C2-O2
2	V	151	GOL	O1-C1-C2-O2
2	X	150	GOL	O1-C1-C2-O2
2	X	150	GOL	O2-C2-C3-O3
2	A	152	GOL	O1-C1-C2-O2
2	B	151	GOL	O2-C2-C3-O3
2	D	151	GOL	O1-C1-C2-O2
2	E	151	GOL	O1-C1-C2-O2
2	H	152	GOL	O1-C1-C2-O2
2	I	152	GOL	O1-C1-C2-O2
2	J	151	GOL	O2-C2-C3-O3
2	M	150	GOL	O1-C1-C2-O2
2	O	152	GOL	O1-C1-C2-O2
2	Q	151	GOL	O2-C2-C3-O3
2	U	150	GOL	O1-C1-C2-O2
2	V	152	GOL	O2-C2-C3-O3
2	D	151	GOL	O2-C2-C3-O3
2	G	152	GOL	O1-C1-C2-O2
2	G	152	GOL	O2-C2-C3-O3
2	K	151	GOL	O2-C2-C3-O3
2	P	152	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	R	152	GOL	O1-C1-C2-O2
2	V	152	GOL	O1-C1-C2-O2
2	L	151	GOL	O1-C1-C2-O2
2	Y	151	GOL	O1-C1-C2-O2
2	B	152	GOL	O1-C1-C2-C3
2	I	152	GOL	O1-C1-C2-C3
2	X	151	GOL	O1-C1-C2-O2
2	C	150	GOL	O2-C2-C3-O3
2	H	151	GOL	O2-C2-C3-O3
2	V	150	GOL	O2-C2-C3-O3
2	Y	150	GOL	O1-C1-C2-C3
2	V	151	GOL	O2-C2-C3-O3
2	F	150	GOL	C1-C2-C3-O3
2	L	150	GOL	C1-C2-C3-O3
2	L	152	GOL	C1-C2-C3-O3
2	D	150	GOL	O1-C1-C2-O2
2	N	151	GOL	O2-C2-C3-O3
2	P	150	GOL	O2-C2-C3-O3
2	P	152	GOL	O2-C2-C3-O3
2	X	152	GOL	O2-C2-C3-O3
2	O	150	GOL	O2-C2-C3-O3
2	K	152	GOL	O1-C1-C2-C3
2	U	151	GOL	O1-C1-C2-O2
2	A	152	GOL	O2-C2-C3-O3
2	B	152	GOL	O1-C1-C2-O2

There are no ring outliers.

53 monomers are involved in 131 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	151	GOL	2	0
2	A	152	GOL	2	0
2	B	151	GOL	3	0
2	X	151	GOL	2	0
2	K	151	GOL	2	0
2	B	152	GOL	2	0
2	A	150	GOL	1	0
2	K	152	GOL	4	0
2	I	152	GOL	2	0
2	N	151	GOL	1	0
2	S	151	GOL	4	0
2	T	151	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	152	GOL	2	0
2	Q	151	GOL	8	0
2	S	150	GOL	2	0
2	P	151	GOL	6	0
2	U	151	GOL	6	0
2	I	151	GOL	2	0
2	F	151	GOL	2	0
2	S	152	GOL	4	0
2	U	152	GOL	2	0
2	F	152	GOL	1	0
2	Y	151	GOL	5	0
2	E	150	GOL	1	0
2	E	151	GOL	1	0
2	H	150	GOL	1	0
2	C	151	GOL	4	0
2	J	151	GOL	2	0
2	O	151	GOL	4	0
2	L	150	GOL	2	0
2	O	152	GOL	4	0
2	E	152	GOL	1	0
2	T	152	GOL	3	0
2	M	152	GOL	2	0
2	X	150	GOL	1	0
2	C	152	GOL	3	0
2	D	151	GOL	4	0
2	G	151	GOL	5	0
2	Q	152	GOL	3	0
2	R	152	GOL	1	0
2	Y	152	GOL	1	0
2	Y	150	GOL	1	0
2	H	151	GOL	2	0
2	D	152	GOL	1	0
2	M	151	GOL	1	0
2	R	151	GOL	5	0
2	L	151	GOL	4	0
2	V	151	GOL	3	0
2	H	152	GOL	2	0
2	L	152	GOL	3	0
2	G	152	GOL	1	0
2	P	152	GOL	1	0
2	V	152	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	O	1
1	C	1
1	D	1
1	P	1
1	L	1
1	Q	1
1	I	1
1	U	1
1	S	1
1	A	1
1	R	1
1	Y	1
1	F	1
1	T	1
1	N	1
1	G	1
1	X	1
1	V	1
1	J	1
1	K	1
1	M	1
1	H	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	141:GLN	C	142:GLN	N	5.77
1	C	141:GLN	C	142:GLN	N	5.67
1	D	141:GLN	C	142:GLN	N	5.59
1	P	141:GLN	C	142:GLN	N	5.45
1	L	141:GLN	C	142:GLN	N	5.26
1	Q	141:GLN	C	142:GLN	N	5.16
1	I	141:GLN	C	142:GLN	N	4.77

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	142:GLN	C	143:GLY	N	4.76
1	U	141:GLN	C	142:GLN	N	4.72
1	S	141:GLN	C	142:GLN	N	4.62
1	A	141:GLN	C	142:GLN	N	4.09
1	R	141:GLN	C	142:GLN	N	4.06
1	Y	141:GLN	C	142:GLN	N	4.03
1	F	141:GLN	C	142:GLN	N	3.91
1	T	141:GLN	C	142:GLN	N	3.73
1	N	141:GLN	C	142:GLN	N	3.40
1	G	141:GLN	C	142:GLN	N	3.31
1	X	141:GLN	C	142:GLN	N	3.28
1	V	141:GLN	C	142:GLN	N	3.23
1	J	141:GLN	C	142:GLN	N	3.21
1	B	141:GLN	C	142:GLN	N	3.07
1	K	141:GLN	C	142:GLN	N	2.59
1	M	141:GLN	C	142:GLN	N	2.01
1	H	141:GLN	C	142:GLN	N	1.87
1	E	141:GLN	C	142:GLN	N	0.83

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.