



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:35 AM UTC

PDB ID : 1GT7 / pdb_00001gt7
Title : L-rhamnulose-1-phosphate aldolase from Escherichia coli
Authors : Kroemer, M.; Schulz, G.E.
Deposited on : 2002-01-14
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

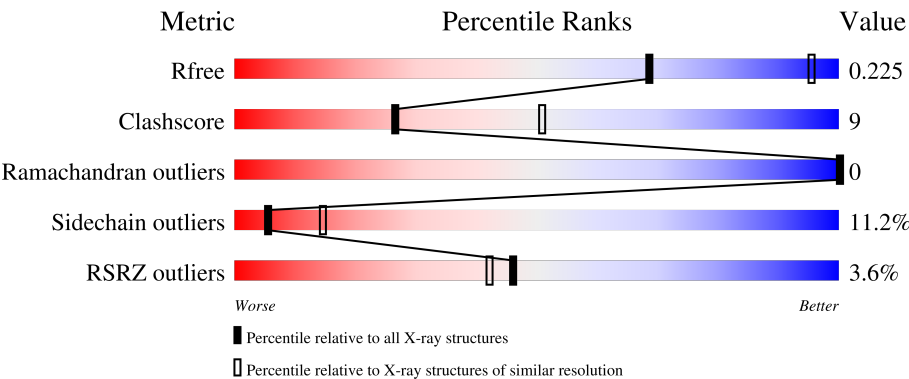
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



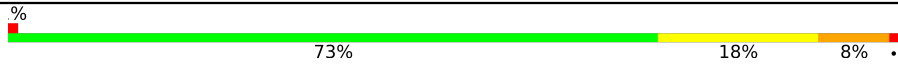
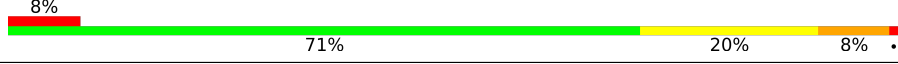
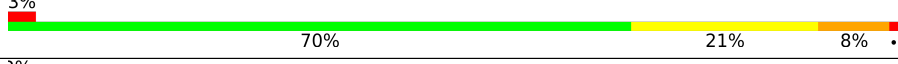
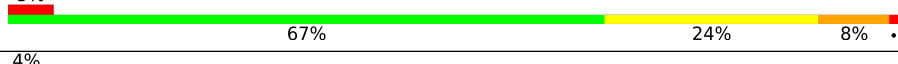
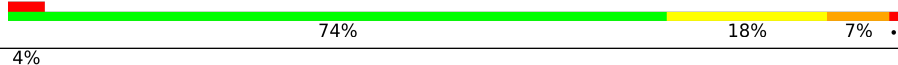
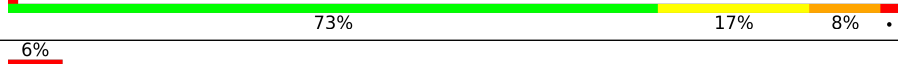
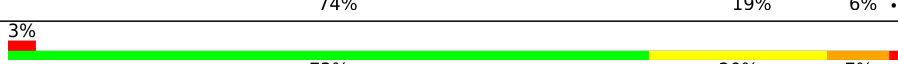
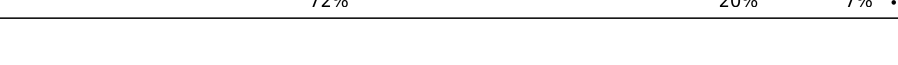
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	274	4% 68% 24% 7%
1	B	274	4% 73% 20% 5%
1	C	274	3% 72% 20% 6%
1	D	274	7% 73% 18% 8%
1	E	274	4% 73% 19% 7%

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Mol	Chain	Length	Quality of chain
1	F	274	
1	G	274	
1	H	274	
1	I	274	
1	J	274	
1	K	274	
1	L	274	
1	M	274	
1	N	274	
1	O	274	
1	P	274	
1	Q	274	
1	R	274	
1	S	274	
1	T	274	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGH	A	300	-	X	-	-
3	PGH	B	300	-	X	-	-
3	PGH	C	300	-	X	-	-
3	PGH	D	300	-	X	-	-
3	PGH	E	300	-	X	-	-
3	PGH	F	300	-	X	-	-
3	PGH	G	300	-	X	-	-
3	PGH	H	300	-	X	-	-
3	PGH	I	300	-	X	-	-
3	PGH	J	300	-	X	-	-
3	PGH	K	300	-	X	-	-
3	PGH	L	300	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PGH	M	300	-	X	-	-
3	PGH	O	300	-	X	-	-
3	PGH	P	300	-	X	-	-
3	PGH	Q	300	-	X	-	-
3	PGH	R	300	-	X	-	-
3	PGH	S	300	-	X	-	-
3	PGH	T	300	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46180 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 RHAMNULOSE-1-PHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	B	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	C	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	D	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	E	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	F	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	G	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	H	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	I	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	J	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	K	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	L	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	M	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	N	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	O	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	P	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	274	Total 2124	C 1358	N 361	O 394	S 11	0	0	0
1	R	274	Total 2124	C 1358	N 361	O 394	S 11	0	0	0
1	S	274	Total 2124	C 1358	N 361	O 394	S 11	0	0	0
1	T	274	Total 2124	C 1358	N 361	O 394	S 11	0	0	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

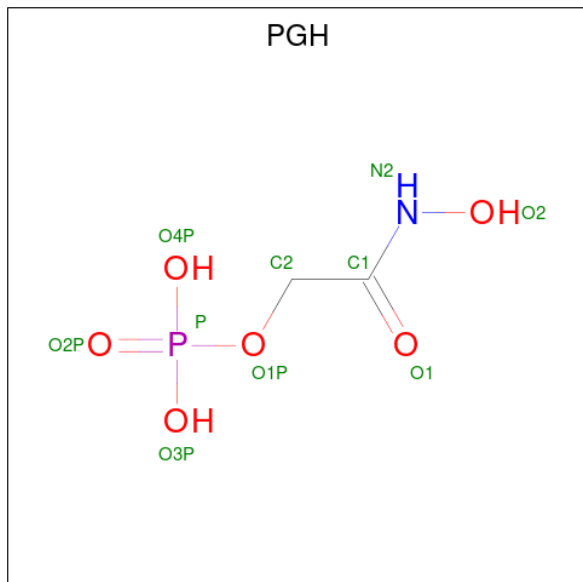
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	J	1	Total 1	Zn 1	0	0
2	K	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0
2	M	1	Total 1	Zn 1	0	0
2	N	1	Total 1	Zn 1	0	0
2	O	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Zn	0	0
			1	1		
2	Q	1	Total	Zn	0	0
			1	1		
2	R	1	Total	Zn	0	0
			1	1		
2	S	1	Total	Zn	0	0
			1	1		
2	T	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHOGLYCOLOHYDROXAMIC ACID (CCD ID: PGH) (formula: $C_2H_6NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	C	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	D	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	E	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	F	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	H	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	I	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	J	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	K	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	L	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	M	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	N	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	O	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	P	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	Q	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	R	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	S	1	Total	C	N	O	P	0	0
			10	2	1	6	1		
3	T	1	Total	C	N	O	P	0	0
			10	2	1	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		
4	B	174	Total	O	0	0
			174	174		
4	C	173	Total	O	0	0
			173	173		
4	D	173	Total	O	0	0
			173	173		
4	E	179	Total	O	0	0
			179	179		

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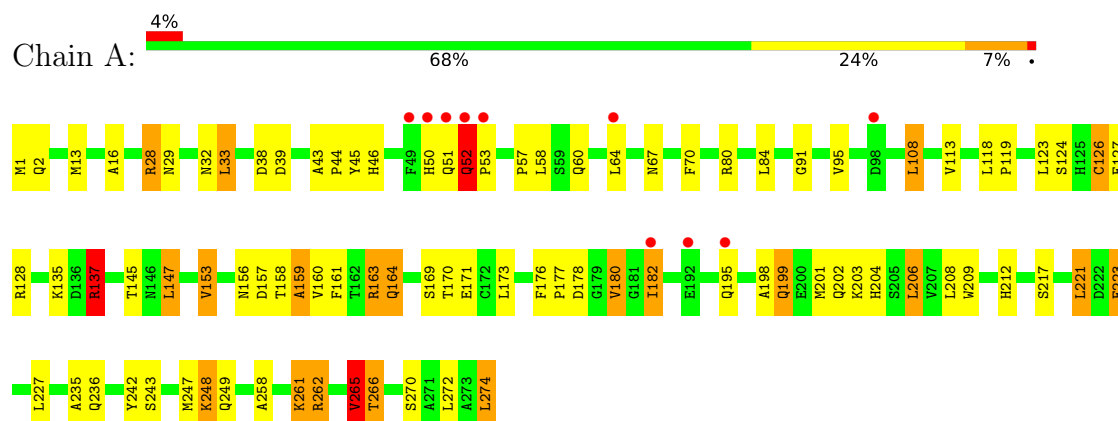
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	174	Total	O	0	0
			174	174		
4	G	176	Total	O	0	0
			176	176		
4	H	171	Total	O	0	0
			171	171		
4	I	177	Total	O	0	0
			177	177		
4	J	178	Total	O	0	0
			178	178		
4	K	177	Total	O	0	0
			177	177		
4	L	167	Total	O	0	0
			167	167		
4	M	183	Total	O	0	0
			183	183		
4	N	170	Total	O	0	0
			170	170		
4	O	175	Total	O	0	0
			175	175		
4	P	167	Total	O	0	0
			167	167		
4	Q	176	Total	O	0	0
			176	176		
4	R	172	Total	O	0	0
			172	172		
4	S	171	Total	O	0	0
			171	171		
4	T	170	Total	O	0	0
			170	170		

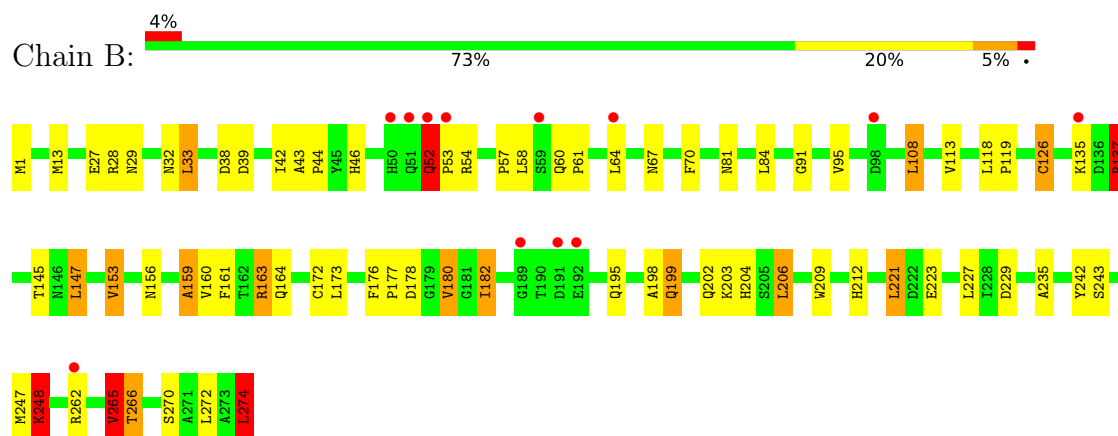
3 Residue-property plots

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

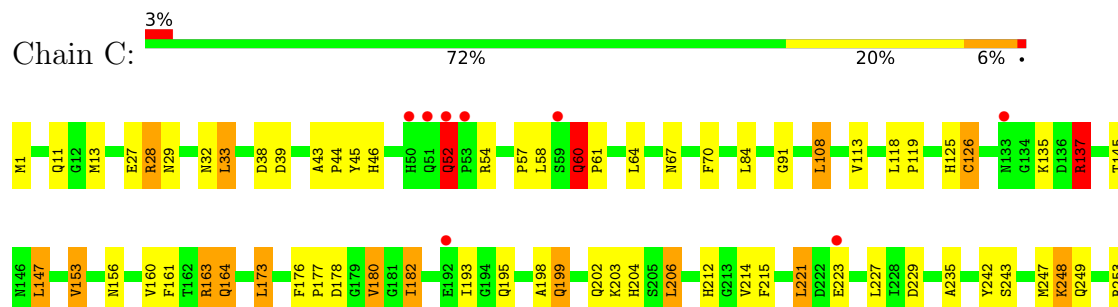
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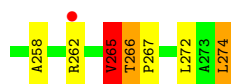


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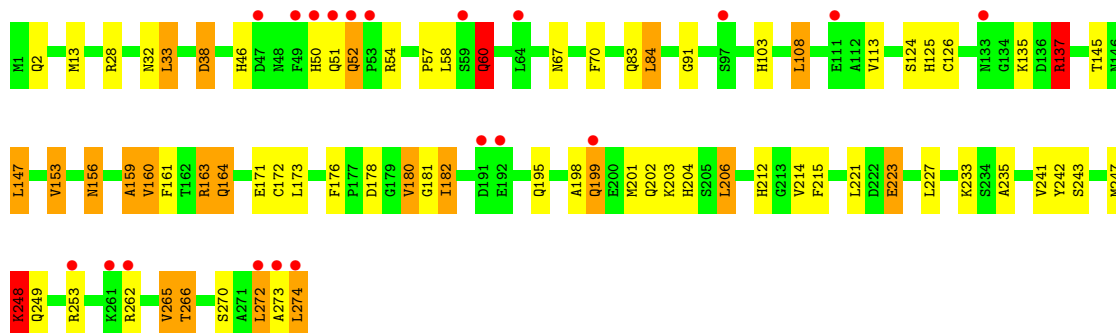
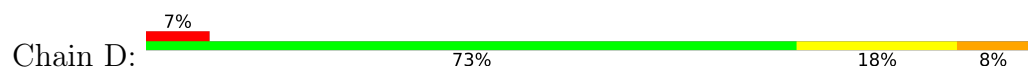


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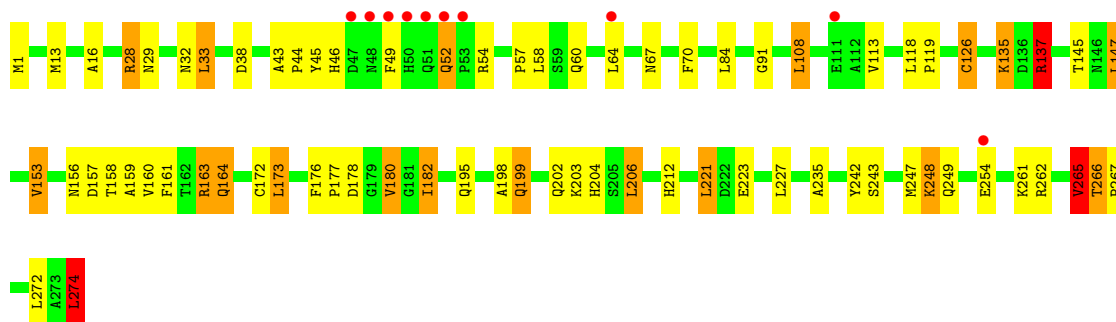
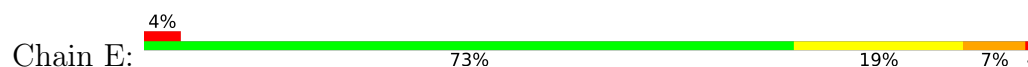




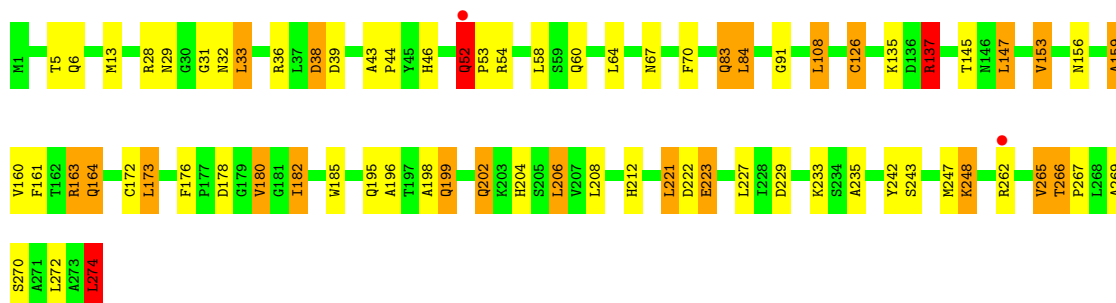
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

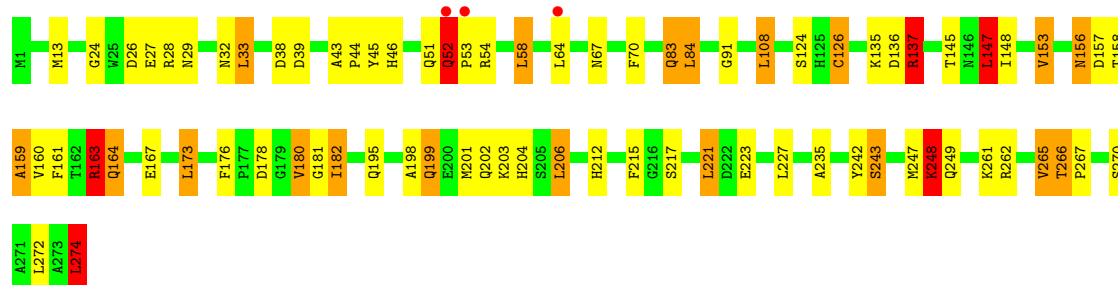


• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

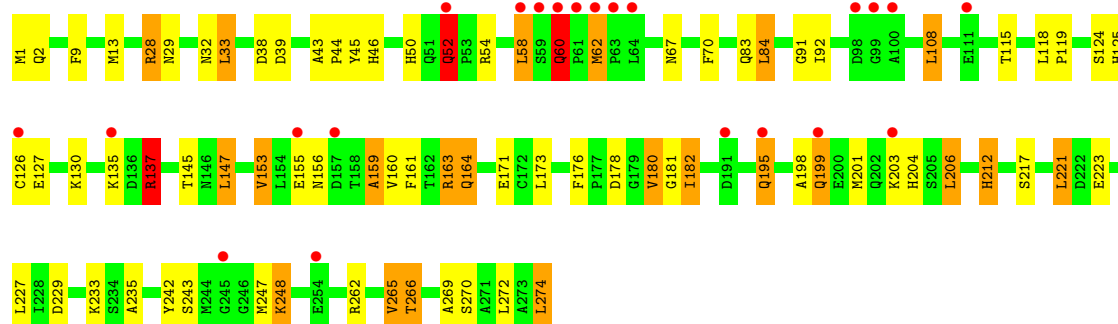


• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

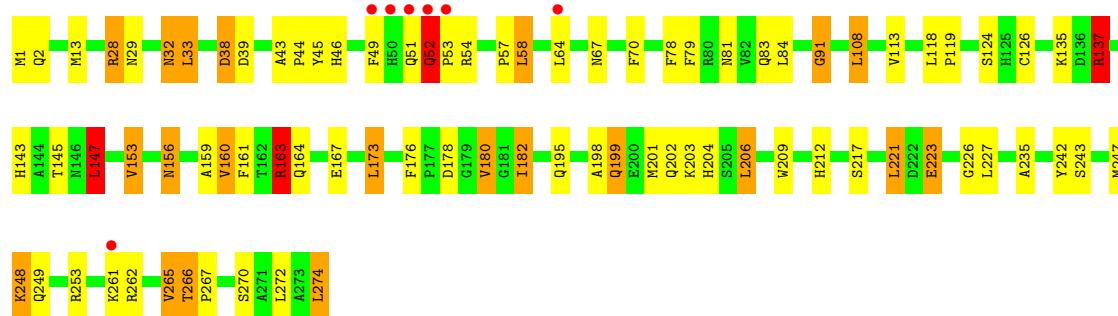




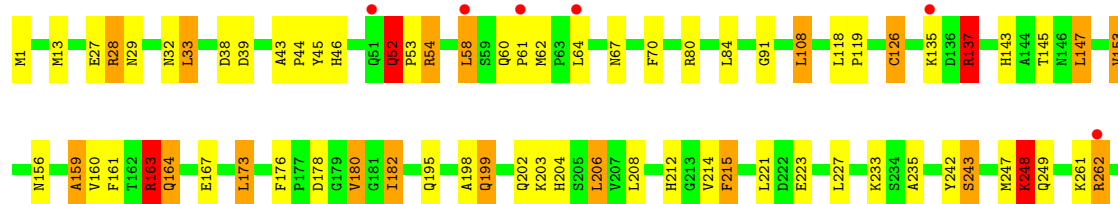
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE



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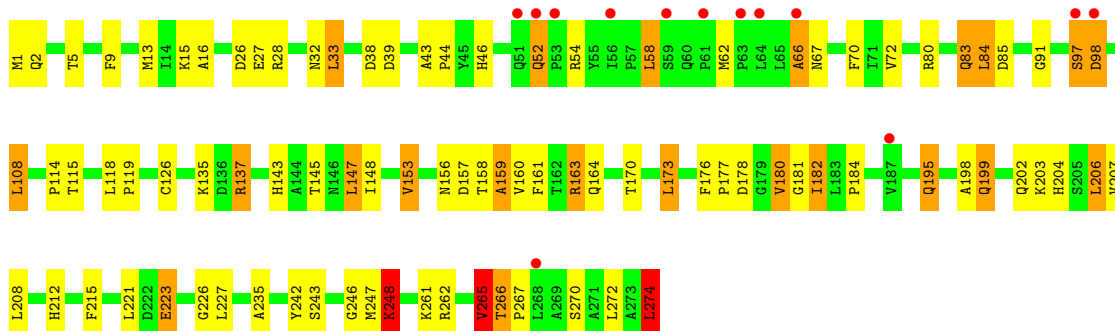
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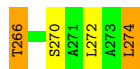
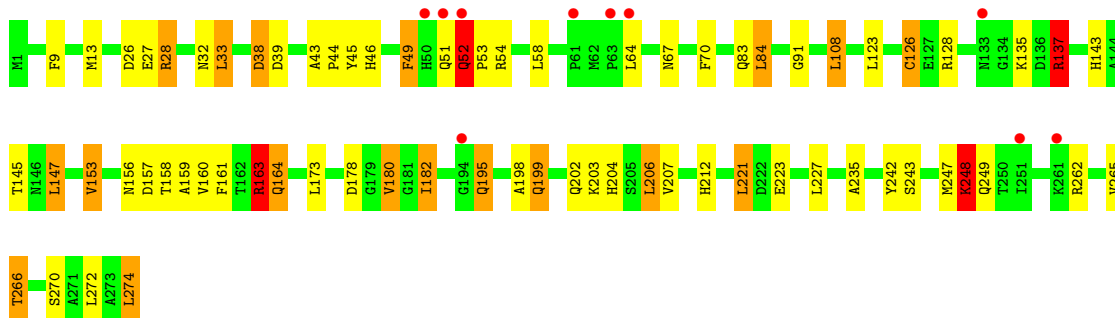
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain K: 5% 67% 24% 8%



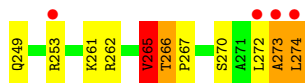
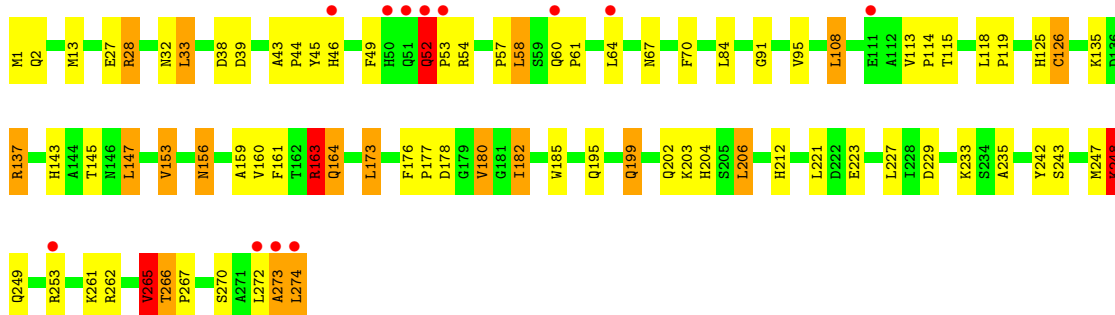
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain L: 4% 74% 18% 7%



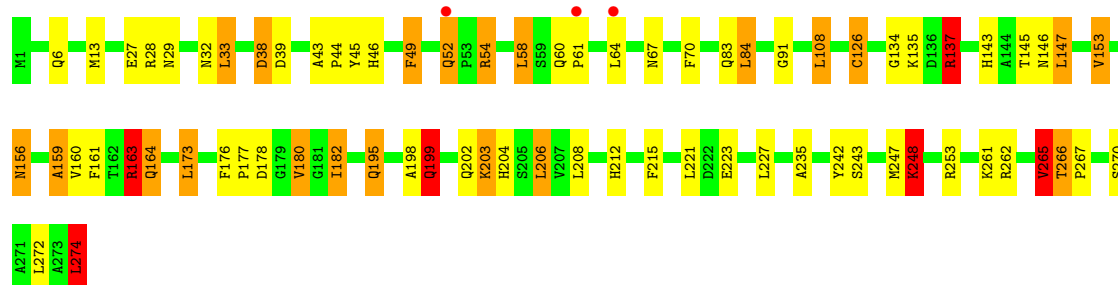
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain M: 4% 70% 22% 7%

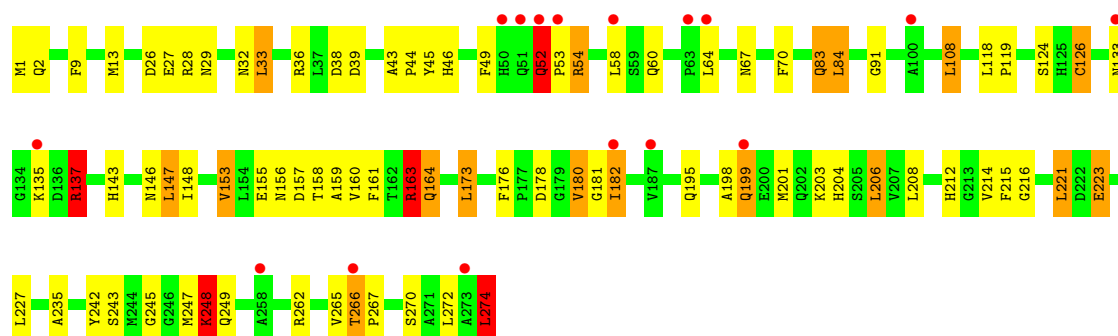


• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

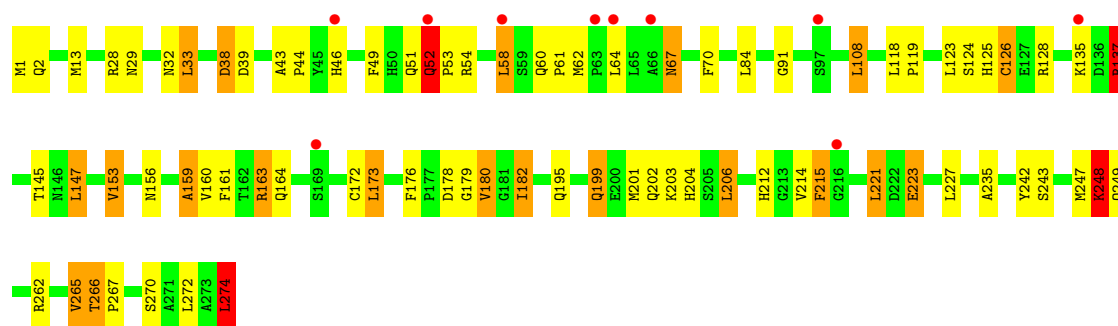
Chain N: % 73% 17% 8%



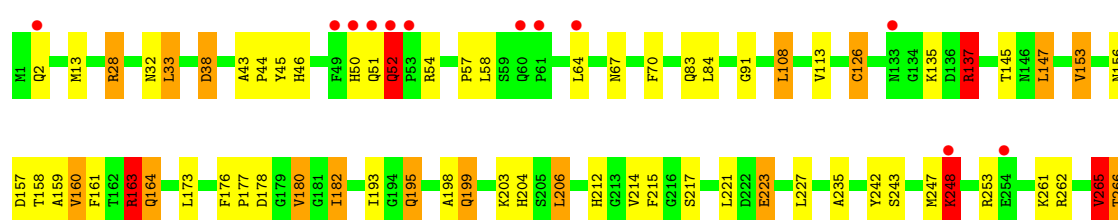
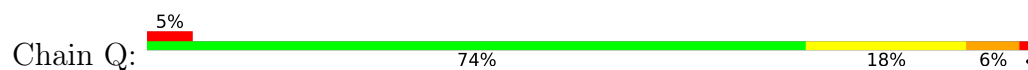
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE



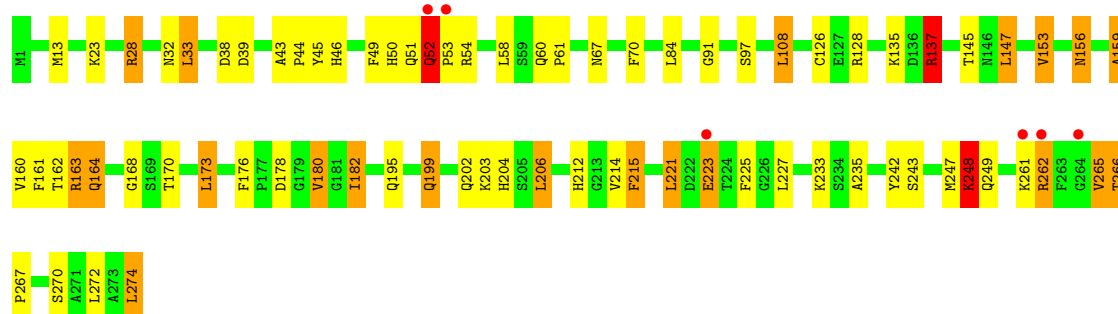
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE





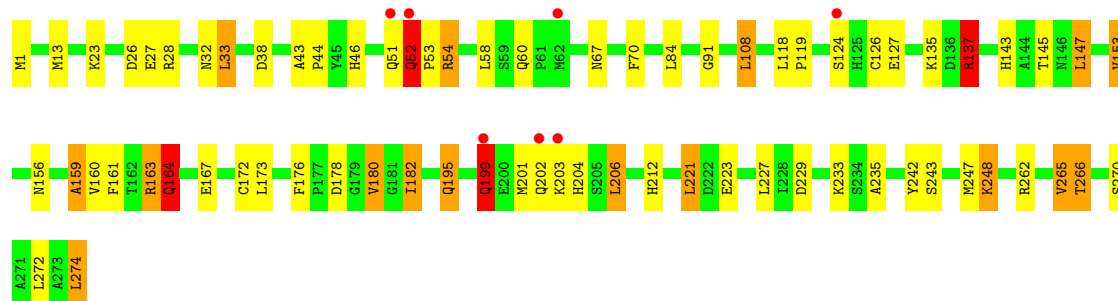
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain R: 2% 73% 19% 8%



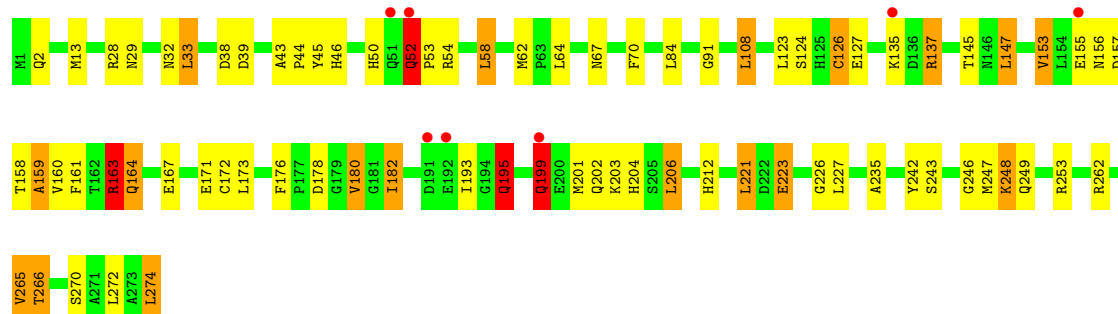
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain S: 3% 74% 19% 6%



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain T: 3% 72% 20% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	225.76Å 225.76Å 285.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.00 – 2.70 44.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (44.00-2.70) 90.3 (44.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.235 0.219 , 0.225	Depositor DCC
R_{free} test set	1036 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	46180	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.05	0/2178	1.74	44/2966 (1.5%)
1	B	1.01	1/2178 (0.0%)	1.71	39/2966 (1.3%)
1	C	1.00	0/2178	1.73	40/2966 (1.3%)
1	D	1.07	0/2178	1.78	48/2966 (1.6%)
1	E	0.99	1/2178 (0.0%)	1.72	37/2966 (1.2%)
1	F	0.95	2/2178 (0.1%)	1.70	40/2966 (1.3%)
1	G	0.95	1/2178 (0.0%)	1.69	42/2966 (1.4%)
1	H	1.04	1/2178 (0.0%)	1.77	49/2966 (1.7%)
1	I	1.00	0/2178	1.71	43/2966 (1.4%)
1	J	1.05	1/2178 (0.0%)	1.69	33/2966 (1.1%)
1	K	1.22	4/2178 (0.2%)	1.79	44/2966 (1.5%)
1	L	1.17	2/2178 (0.1%)	1.73	35/2966 (1.2%)
1	M	0.99	1/2178 (0.0%)	1.72	36/2966 (1.2%)
1	N	1.06	1/2178 (0.0%)	1.70	40/2966 (1.3%)
1	O	1.24	2/2178 (0.1%)	1.76	42/2966 (1.4%)
1	P	1.12	1/2178 (0.0%)	1.69	40/2966 (1.3%)
1	Q	1.05	1/2178 (0.0%)	1.73	41/2966 (1.4%)
1	R	1.01	1/2178 (0.0%)	1.71	44/2966 (1.5%)
1	S	0.99	2/2178 (0.1%)	1.72	37/2966 (1.2%)
1	T	0.99	0/2178	1.72	43/2966 (1.4%)
All	All	1.05	22/43560 (0.1%)	1.73	817/59320 (1.4%)

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	D	0	1
1	F	0	1
1	I	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	N	0	1
1	P	0	1
1	Q	0	1
All	All	0	7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	274	LEU	C-OXT	9.70	1.43	1.23
1	P	274	LEU	C-OXT	9.43	1.42	1.23
1	B	274	LEU	C-OXT	9.18	1.42	1.23
1	N	274	LEU	C-OXT	9.09	1.41	1.23
1	K	274	LEU	C-OXT	8.49	1.40	1.23
1	Q	274	LEU	C-OXT	6.83	1.37	1.23
1	G	274	LEU	C-OXT	6.33	1.36	1.23
1	F	274	LEU	C-OXT	6.30	1.36	1.23
1	H	212	HIS	ND1-CE1	-6.19	1.26	1.32
1	J	143	HIS	ND1-CE1	6.17	1.38	1.32
1	L	207	VAL	C-O	6.10	1.30	1.24
1	K	72	VAL	C-O	6.04	1.30	1.23
1	S	26	ASP	CA-CB	6.04	1.57	1.53
1	E	274	LEU	C-OXT	5.91	1.35	1.23
1	K	80	ARG	NE-CZ	5.86	1.39	1.33
1	O	216	GLY	N-CA	5.56	1.51	1.45
1	L	143	HIS	CE1-NE2	5.35	1.37	1.32
1	S	199	GLN	CD-NE2	5.29	1.44	1.33
1	K	246	GLY	N-CA	5.27	1.50	1.45
1	R	162	THR	C-N	5.13	1.40	1.33
1	F	222	ASP	N-CA	-5.08	1.40	1.46
1	M	273	ALA	C-O	5.01	1.30	1.24

All (817) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	52	GLN	CB-CG-CD	10.59	130.59	112.60
1	N	52	GLN	CB-CG-CD	10.56	130.55	112.60
1	F	52	GLN	CB-CG-CD	10.37	130.22	112.60
1	H	52	GLN	CB-CG-CD	9.87	129.38	112.60
1	F	266	THR	CB-CA-C	9.76	121.00	110.17
1	M	266	THR	CB-CA-C	9.56	120.08	110.33
1	C	163	ARG	NE-CZ-NH2	-9.53	110.62	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	52	GLN	CB-CG-CD	9.53	128.80	112.60
1	B	52	GLN	CB-CG-CD	9.48	128.71	112.60
1	Q	52	GLN	CB-CG-CD	9.46	128.69	112.60
1	H	266	THR	CB-CA-C	9.42	120.63	110.17
1	M	163	ARG	NE-CZ-NH1	9.26	130.76	121.50
1	R	52	GLN	CB-CG-CD	9.22	128.28	112.60
1	D	266	THR	CB-CA-C	9.21	119.72	110.33
1	K	266	THR	CB-CA-C	9.18	120.36	110.17
1	P	266	THR	CB-CA-C	9.16	120.34	110.17
1	E	266	THR	CB-CA-C	9.11	120.28	110.17
1	O	266	THR	CB-CA-C	9.08	120.25	110.17
1	S	199	GLN	CB-CG-CD	-9.08	97.16	112.60
1	K	52	GLN	CB-CG-CD	9.07	128.02	112.60
1	P	266	THR	CA-C-O	9.05	127.92	119.59
1	S	52	GLN	CB-CG-CD	9.04	127.97	112.60
1	G	266	THR	CB-CA-C	8.99	119.50	110.33
1	B	266	THR	CB-CA-C	8.93	120.08	110.17
1	T	266	THR	CB-CA-C	8.91	120.06	110.17
1	J	52	GLN	CB-CG-CD	8.90	127.73	112.60
1	D	266	THR	CA-C-O	8.84	127.68	119.99
1	D	163	ARG	NE-CZ-NH2	-8.81	111.27	119.20
1	A	52	GLN	CB-CG-CD	8.80	127.55	112.60
1	D	176	PHE	CA-CB-CG	8.76	122.56	113.80
1	D	52	GLN	CB-CG-CD	8.76	127.50	112.60
1	A	262	ARG	NH1-CZ-NH2	-8.66	108.03	119.30
1	O	52	GLN	CB-CG-CD	8.64	127.29	112.60
1	L	266	THR	CB-CA-C	8.63	119.75	110.17
1	S	266	THR	CB-CA-C	8.62	119.73	110.17
1	E	38	ASP	CB-CA-C	-8.59	95.08	110.36
1	C	266	THR	CB-CA-C	8.56	119.68	110.17
1	I	266	THR	CB-CA-C	8.52	119.63	110.17
1	I	52	GLN	CB-CG-CD	8.51	127.07	112.60
1	H	70	PHE	CA-CB-CG	8.48	122.28	113.80
1	S	266	THR	CA-C-O	8.47	127.38	119.59
1	D	70	PHE	CA-CB-CG	8.47	122.27	113.80
1	R	70	PHE	CA-CB-CG	8.45	122.25	113.80
1	D	262	ARG	NH1-CZ-NH2	-8.44	108.33	119.30
1	B	70	PHE	CA-CB-CG	8.41	122.21	113.80
1	G	52	GLN	CB-CG-CD	8.39	126.87	112.60
1	E	70	PHE	CA-CB-CG	8.38	122.18	113.80
1	E	52	GLN	CB-CG-CD	8.35	126.80	112.60
1	S	199	GLN	N-CA-CB	-8.35	97.91	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	66	ALA	CB-CA-C	8.34	124.54	109.62
1	Q	266	THR	CB-CA-C	8.32	119.41	110.17
1	C	176	PHE	CA-CB-CG	8.30	122.10	113.80
1	H	38	ASP	CB-CA-C	-8.26	95.66	110.36
1	Q	70	PHE	CA-CB-CG	8.25	122.05	113.80
1	J	266	THR	CB-CA-C	8.13	119.19	110.17
1	G	38	ASP	CB-CA-C	-8.11	95.92	110.36
1	I	266	THR	CA-C-O	8.10	127.04	119.59
1	M	163	ARG	NE-CZ-NH2	-8.08	111.92	119.20
1	R	266	THR	CA-C-O	8.06	127.00	119.59
1	T	199	GLN	OE1-CD-NE2	8.02	130.62	122.60
1	G	266	THR	CA-C-O	8.00	126.95	119.99
1	C	262	ARG	NH1-CZ-NH2	-7.99	108.92	119.30
1	C	52	GLN	CB-CG-CD	7.98	126.17	112.60
1	N	266	THR	CB-CA-C	7.98	119.03	110.17
1	H	199	GLN	CB-CG-CD	-7.98	99.04	112.60
1	G	70	PHE	CA-CB-CG	7.97	121.77	113.80
1	P	153	VAL	N-CA-CB	-7.97	99.30	111.57
1	C	28	ARG	CB-CA-C	-7.92	107.43	116.54
1	R	266	THR	CB-CA-C	7.91	118.95	110.17
1	H	262	ARG	NH1-CZ-NH2	-7.90	109.03	119.30
1	O	38	ASP	CB-CA-C	-7.90	95.38	110.24
1	J	38	ASP	CB-CA-C	-7.87	95.44	110.24
1	T	38	ASP	CB-CA-C	-7.87	96.35	110.36
1	A	70	PHE	CA-CB-CG	7.86	121.66	113.80
1	Q	38	ASP	CB-CA-C	-7.86	96.37	110.36
1	S	164	GLN	OE1-CD-NE2	-7.83	114.77	122.60
1	K	181	GLY	CA-C-O	-7.83	114.44	121.64
1	R	38	ASP	CB-CA-C	-7.83	96.43	110.36
1	T	52	GLN	CB-CG-CD	7.82	125.90	112.60
1	S	70	PHE	CA-CB-CG	7.80	121.60	113.80
1	L	262	ARG	NH1-CZ-NH2	-7.80	109.16	119.30
1	B	38	ASP	CB-CA-C	-7.78	96.51	110.36
1	M	70	PHE	CA-CB-CG	7.78	121.58	113.80
1	M	52	GLN	CB-CG-CD	7.78	125.83	112.60
1	C	38	ASP	CB-CA-C	-7.78	95.61	110.24
1	N	38	ASP	CB-CA-C	-7.78	96.52	110.36
1	M	38	ASP	CB-CA-C	-7.77	95.64	110.24
1	A	38	ASP	CB-CA-C	-7.74	96.59	110.36
1	B	266	THR	CA-C-O	7.74	126.71	119.59
1	L	199	GLN	CB-CG-CD	-7.71	99.49	112.60
1	O	266	THR	CA-C-O	7.71	126.69	119.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	253	ARG	NE-CZ-NH1	7.71	129.22	121.50
1	M	176	PHE	CA-CB-CG	7.70	121.50	113.80
1	L	39	ASP	CA-CB-CG	-7.68	104.92	112.60
1	F	70	PHE	CA-CB-CG	7.67	121.47	113.80
1	N	266	THR	CA-C-O	7.67	126.64	119.59
1	E	52	GLN	OE1-CD-NE2	-7.66	114.94	122.60
1	L	38	ASP	CB-CA-C	-7.65	95.85	110.24
1	A	198	ALA	CA-C-O	7.65	128.66	120.55
1	P	38	ASP	CB-CA-C	-7.64	96.75	110.36
1	Q	195	GLN	OE1-CD-NE2	7.64	130.24	122.60
1	A	266	THR	CB-CA-C	7.63	118.64	110.17
1	D	262	ARG	NE-CZ-NH2	7.60	126.04	119.20
1	D	38	ASP	CB-CA-C	-7.57	96.89	110.36
1	S	38	ASP	CB-CA-C	-7.56	96.90	110.36
1	M	248	LYS	CB-CA-C	7.54	123.01	109.29
1	T	266	THR	CA-C-O	7.53	126.52	119.59
1	D	52	GLN	CB-CA-C	-7.51	100.97	110.96
1	D	60	GLN	OE1-CD-NE2	7.50	130.10	122.60
1	L	137	ARG	CD-NE-CZ	7.49	134.89	124.40
1	K	198	ALA	CA-C-O	7.49	128.49	120.55
1	F	38	ASP	CB-CA-C	-7.49	97.03	110.36
1	S	221	LEU	O-C-N	-7.48	114.36	122.07
1	A	176	PHE	CA-CB-CG	7.48	121.28	113.80
1	E	176	PHE	CA-CB-CG	7.47	121.27	113.80
1	C	198	ALA	CA-C-O	7.44	128.44	120.55
1	H	159	ALA	CA-C-O	-7.44	113.03	120.70
1	G	137	ARG	CD-NE-CZ	7.44	134.81	124.40
1	B	198	ALA	CA-C-O	7.43	128.42	120.55
1	I	38	ASP	CB-CA-C	-7.42	97.16	110.36
1	F	159	ALA	CA-C-O	-7.39	112.59	120.42
1	I	45	TYR	N-CA-C	7.39	120.92	112.57
1	K	266	THR	CA-C-O	7.38	126.38	119.59
1	F	137	ARG	CD-NE-CZ	7.37	134.71	124.40
1	A	39	ASP	CA-CB-CG	-7.36	105.24	112.60
1	J	199	GLN	CB-CG-CD	-7.35	100.10	112.60
1	L	51	GLN	CA-C-N	7.35	131.96	123.21
1	L	51	GLN	C-N-CA	7.35	131.96	123.21
1	Q	159	ALA	CA-C-O	-7.33	112.66	120.42
1	T	176	PHE	CA-CB-CG	7.30	121.10	113.80
1	S	159	ALA	CA-C-O	-7.29	112.70	120.42
1	I	39	ASP	CA-CB-CG	-7.28	105.32	112.60
1	J	163	ARG	NE-CZ-NH2	-7.28	112.65	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	266	THR	CA-C-O	7.27	126.28	119.59
1	B	176	PHE	CA-CB-CG	7.26	121.06	113.80
1	J	159	ALA	CA-C-O	-7.26	112.73	120.42
1	K	38	ASP	CB-CA-C	-7.25	97.47	110.36
1	S	199	GLN	OE1-CD-NE2	7.25	129.84	122.60
1	T	70	PHE	CA-CB-CG	7.23	121.03	113.80
1	J	145	THR	N-CA-C	7.21	119.82	111.02
1	L	45	TYR	N-CA-C	7.20	120.93	112.72
1	E	262	ARG	NE-CZ-NH2	7.20	125.68	119.20
1	P	70	PHE	CA-CB-CG	7.20	121.00	113.80
1	E	137	ARG	CD-NE-CZ	7.17	134.44	124.40
1	M	248	LYS	CA-C-O	7.16	127.02	119.14
1	S	199	GLN	CG-CD-NE2	-7.16	105.66	116.40
1	Q	248	LYS	CB-CA-C	7.16	122.31	109.29
1	R	145	THR	N-CA-C	7.16	119.75	111.02
1	M	262	ARG	NH1-CZ-NH2	-7.15	110.01	119.30
1	S	176	PHE	CA-CB-CG	7.14	120.94	113.80
1	J	39	ASP	CA-CB-CG	-7.13	105.47	112.60
1	I	83	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	Q	52	GLN	CB-CA-C	-7.11	101.50	110.96
1	C	70	PHE	CA-CB-CG	7.10	120.90	113.80
1	E	199	GLN	CB-CG-CD	-7.07	100.58	112.60
1	F	176	PHE	CA-CB-CG	7.07	120.87	113.80
1	O	143	HIS	CA-CB-CG	-7.06	106.74	113.80
1	R	199	GLN	CB-CG-CD	-7.04	100.63	112.60
1	G	45	TYR	N-CA-C	7.02	120.50	112.57
1	A	199	GLN	CB-CG-CD	-7.01	100.68	112.60
1	Q	137	ARG	CD-NE-CZ	7.01	134.22	124.40
1	E	153	VAL	N-CA-CB	-7.01	100.78	111.57
1	G	176	PHE	CA-CB-CG	7.00	120.80	113.80
1	L	70	PHE	CA-CB-CG	7.00	120.80	113.80
1	H	125	HIS	CA-C-O	6.99	128.16	120.82
1	M	199	GLN	CB-CG-CD	-6.99	100.72	112.60
1	N	176	PHE	CA-CB-CG	6.97	120.78	113.80
1	M	45	TYR	N-CA-C	6.97	120.67	112.72
1	H	50	HIS	CA-CB-CG	6.96	120.76	113.80
1	F	198	ALA	CA-C-O	6.96	127.93	120.55
1	F	262	ARG	NH1-CZ-NH2	-6.95	110.26	119.30
1	J	70	PHE	CA-CB-CG	6.94	120.74	113.80
1	E	198	ALA	CA-C-O	6.92	127.89	120.55
1	P	262	ARG	NH1-CZ-NH2	-6.90	110.33	119.30
1	R	225	PHE	CA-C-N	6.89	127.63	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	225	PHE	C-N-CA	6.89	127.63	119.98
1	E	249	GLN	N-CA-CB	6.89	123.17	111.66
1	Q	176	PHE	CA-CB-CG	6.87	120.67	113.80
1	C	39	ASP	CA-CB-CG	-6.87	105.73	112.60
1	F	266	THR	CA-C-O	6.87	125.91	119.59
1	O	249	GLN	N-CA-CB	6.85	123.11	111.66
1	O	45	TYR	N-CA-C	6.85	120.31	112.57
1	G	198	ALA	CA-C-O	6.83	127.79	120.55
1	C	137	ARG	CD-NE-CZ	6.82	133.95	124.40
1	N	137	ARG	CD-NE-CZ	6.82	133.94	124.40
1	R	164	GLN	CA-CB-CG	6.78	127.67	114.10
1	O	70	PHE	CA-CB-CG	6.78	120.58	113.80
1	L	145	THR	N-CA-C	6.77	119.28	111.02
1	H	60	GLN	O-C-N	-6.77	116.56	121.84
1	B	262	ARG	NH1-CZ-NH2	-6.77	110.50	119.30
1	H	199	GLN	OE1-CD-NE2	6.77	129.37	122.60
1	N	70	PHE	CA-CB-CG	6.76	120.56	113.80
1	H	199	GLN	CG-CD-NE2	-6.75	106.27	116.40
1	G	248	LYS	CB-CA-C	6.75	121.57	109.29
1	F	153	VAL	N-CA-CB	-6.74	100.11	111.23
1	I	248	LYS	N-CA-C	-6.73	105.22	113.50
1	I	70	PHE	CA-CB-CG	6.71	120.51	113.80
1	F	199	GLN	CB-CG-CD	-6.71	101.19	112.60
1	C	60	GLN	OE1-CD-NE2	6.69	129.29	122.60
1	Q	182	ILE	CB-CA-C	-6.69	100.73	110.63
1	E	126	CYS	CB-CA-C	6.69	121.38	110.88
1	J	198	ALA	CA-C-O	6.68	127.63	120.55
1	I	51	GLN	CA-C-N	6.67	131.15	123.21
1	I	51	GLN	C-N-CA	6.67	131.15	123.21
1	T	172	CYS	N-CA-C	6.67	118.55	111.28
1	G	262	ARG	NH1-CZ-NH2	-6.66	110.65	119.30
1	N	54	ARG	CD-NE-CZ	6.65	133.71	124.40
1	Q	52	GLN	OE1-CD-NE2	-6.65	115.95	122.60
1	R	262	ARG	NE-CZ-NH2	6.65	125.18	119.20
1	D	248	LYS	O-C-N	-6.63	113.60	122.49
1	H	153	VAL	N-CA-CB	-6.62	100.31	111.23
1	E	28	ARG	CB-CA-C	-6.61	108.93	116.54
1	A	137	ARG	CD-NE-CZ	6.61	133.65	124.40
1	B	248	LYS	CA-C-O	6.60	126.40	119.14
1	E	262	ARG	NH1-CZ-NH2	-6.60	110.72	119.30
1	N	182	ILE	CB-CA-C	-6.60	101.00	110.83
1	I	262	ARG	NH1-CZ-NH2	-6.59	110.74	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	262	ARG	NH1-CZ-NH2	-6.58	110.75	119.30
1	Q	199	GLN	CB-CG-CD	-6.58	101.41	112.60
1	P	145	THR	N-CA-C	6.58	119.04	111.02
1	K	143	HIS	CA-CB-CG	-6.58	107.22	113.80
1	I	137	ARG	CD-NE-CZ	6.57	133.60	124.40
1	H	266	THR	CA-C-O	6.56	125.63	119.59
1	C	199	GLN	CB-CG-CD	-6.56	101.45	112.60
1	N	6	GLN	OE1-CD-NE2	6.54	129.14	122.60
1	R	221	LEU	O-C-N	-6.53	115.35	122.07
1	I	199	GLN	CB-CG-CD	-6.53	101.51	112.60
1	T	262	ARG	NH1-CZ-NH2	-6.52	110.82	119.30
1	I	182	ILE	CB-CA-C	-6.52	100.98	110.63
1	R	126	CYS	CB-CA-C	6.52	121.11	110.88
1	A	145	THR	N-CA-C	6.52	118.97	111.02
1	Q	248	LYS	N-CA-C	-6.51	105.49	113.50
1	P	176	PHE	CA-CB-CG	6.50	120.30	113.80
1	N	153	VAL	N-CA-CB	-6.49	100.52	111.23
1	A	248	LYS	CA-C-O	6.49	126.28	119.14
1	N	199	GLN	CB-CG-CD	-6.49	101.57	112.60
1	P	182	ILE	CB-CA-C	-6.48	101.17	110.83
1	K	67	ASN	CA-CB-CG	-6.47	106.13	112.60
1	E	29	ASN	OD1-CG-ND2	6.47	129.07	122.60
1	A	182	ILE	N-CA-CB	6.45	120.31	111.41
1	N	143	HIS	CA-CB-CG	-6.45	107.35	113.80
1	R	159	ALA	CA-C-O	-6.45	113.59	120.42
1	T	193	ILE	CA-C-N	6.44	127.09	119.94
1	T	193	ILE	C-N-CA	6.44	127.09	119.94
1	F	6	GLN	OE1-CD-NE2	6.43	129.03	122.60
1	K	182	ILE	CB-CA-C	-6.43	101.25	110.83
1	J	54	ARG	CD-NE-CZ	6.42	133.38	124.40
1	J	45	TYR	N-CA-C	6.40	120.39	112.59
1	K	83	GLN	OE1-CD-NE2	6.38	128.98	122.60
1	P	51	GLN	CA-C-N	6.38	130.81	123.21
1	P	51	GLN	C-N-CA	6.38	130.81	123.21
1	A	236	GLN	OE1-CD-NE2	-6.38	116.22	122.60
1	M	145	THR	N-CA-C	6.37	118.79	111.02
1	C	258	ALA	CA-C-N	6.37	128.71	120.44
1	C	258	ALA	C-N-CA	6.37	128.71	120.44
1	D	272	LEU	O-C-N	-6.36	113.81	122.33
1	O	248	LYS	CB-CA-C	6.35	120.85	109.29
1	C	125	HIS	CA-C-O	6.34	127.48	120.82
1	P	137	ARG	CD-NE-CZ	6.34	133.28	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	148	ILE	O-C-N	-6.34	115.70	121.91
1	C	262	ARG	NE-CZ-NH2	6.34	124.90	119.20
1	J	137	ARG	CD-NE-CZ	6.34	133.27	124.40
1	H	176	PHE	CA-CB-CG	6.33	120.13	113.80
1	H	265	VAL	CB-CA-C	6.32	120.23	110.50
1	R	262	ARG	NH1-CZ-NH2	-6.32	111.09	119.30
1	C	249	GLN	N-CA-CB	6.30	122.19	111.66
1	J	266	THR	CA-C-O	6.30	125.39	119.59
1	R	52	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	R	223	GLU	CG-CD-OE2	-6.29	103.93	118.40
1	O	199	GLN	CB-CG-CD	-6.28	101.92	112.60
1	Q	38	ASP	CA-CB-CG	6.28	118.88	112.60
1	I	156	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	J	126	CYS	CB-CA-C	6.27	121.20	110.79
1	I	153	VAL	N-CA-CB	-6.26	100.89	111.23
1	A	223	GLU	CG-CD-OE2	-6.26	104.00	118.40
1	A	249	GLN	N-CA-CB	6.26	122.11	111.66
1	E	45	TYR	N-CA-C	6.25	120.22	112.59
1	G	156	ASN	OD1-CG-ND2	-6.25	116.35	122.60
1	B	199	GLN	CB-CG-CD	-6.25	101.98	112.60
1	S	54	ARG	CD-NE-CZ	6.24	133.14	124.40
1	G	39	ASP	CA-CB-CG	-6.24	106.36	112.60
1	M	159	ALA	CA-C-O	-6.24	113.81	120.42
1	H	145	THR	N-CA-C	6.22	118.61	111.02
1	J	153	VAL	N-CA-CB	-6.21	100.99	111.23
1	A	163	ARG	NE-CZ-NH2	-6.21	113.61	119.20
1	S	153	VAL	N-CA-CB	-6.21	100.99	111.23
1	K	248	LYS	N-CA-C	-6.20	105.88	113.50
1	C	266	THR	CA-C-O	6.19	125.29	119.59
1	R	163	ARG	NE-CZ-NH2	-6.18	113.64	119.20
1	B	248	LYS	CB-CA-C	6.18	120.53	109.29
1	I	248	LYS	CB-CA-C	6.18	120.53	109.29
1	O	39	ASP	CA-CB-CG	-6.18	106.42	112.60
1	M	249	GLN	N-CA-CB	6.17	121.97	111.66
1	G	159	ALA	CA-C-O	-6.17	113.88	120.42
1	S	265	VAL	CB-CA-C	6.16	119.99	110.50
1	D	125	HIS	CA-C-O	6.16	127.29	120.82
1	M	262	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	K	5	THR	CA-C-O	-6.15	112.05	119.49
1	L	163	ARG	NE-CZ-NH2	-6.15	113.66	119.20
1	K	38	ASP	CA-CB-CG	6.15	118.75	112.60
1	B	248	LYS	O-C-N	-6.14	114.26	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	153	VAL	N-CA-CB	-6.13	101.11	111.23
1	S	60	GLN	OE1-CD-NE2	6.13	128.73	122.60
1	K	248	LYS	CB-CA-C	6.13	120.44	109.29
1	T	137	ARG	CD-NE-CZ	6.13	132.98	124.40
1	D	272	LEU	CA-C-O	6.12	127.02	119.79
1	Q	83	GLN	OE1-CD-NE2	6.12	128.72	122.60
1	R	170	THR	CA-C-O	-6.11	114.03	120.63
1	B	163	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	M	156	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	O	38	ASP	CA-CB-CG	6.11	118.71	112.60
1	P	199	GLN	CB-CG-CD	-6.11	102.22	112.60
1	E	164	GLN	CA-CB-CG	6.10	126.29	114.10
1	M	126	CYS	CB-CA-C	6.10	120.56	110.81
1	J	215	PHE	CA-C-N	-6.10	116.34	121.58
1	J	215	PHE	C-N-CA	-6.10	116.34	121.58
1	A	126	CYS	CB-CA-C	6.09	120.45	110.88
1	B	95	VAL	CA-C-O	-6.09	114.71	121.23
1	J	182	ILE	CB-CA-C	-6.09	101.61	110.63
1	G	199	GLN	CB-CG-CD	-6.09	102.25	112.60
1	K	199	GLN	CB-CG-CD	-6.09	102.24	112.60
1	O	126	CYS	CB-CA-C	6.08	120.43	110.88
1	A	153	VAL	N-CA-CB	-6.08	101.19	111.23
1	M	153	VAL	N-CA-CB	-6.08	101.20	111.23
1	N	262	ARG	NH1-CZ-NH2	-6.08	111.40	119.30
1	O	163	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	D	248	LYS	CB-CA-C	6.08	120.35	109.29
1	E	49	PHE	CA-CB-CG	-6.07	107.73	113.80
1	G	51	GLN	CA-C-N	6.07	130.43	123.21
1	G	51	GLN	C-N-CA	6.07	130.43	123.21
1	P	159	ALA	CA-C-O	-6.06	114.45	120.70
1	R	54	ARG	CD-NE-CZ	6.06	132.89	124.40
1	T	164	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	G	182	ILE	CB-CA-C	-6.06	101.81	110.83
1	E	182	ILE	CB-CA-C	-6.05	101.67	110.63
1	E	159	ALA	CA-C-O	-6.05	114.00	120.42
1	Q	262	ARG	NH1-CZ-NH2	-6.05	111.44	119.30
1	R	137	ARG	CD-NE-CZ	6.04	132.86	124.40
1	N	159	ALA	CA-C-O	-6.03	114.03	120.42
1	N	39	ASP	CA-CB-CG	-6.03	106.57	112.60
1	C	145	THR	N-CA-C	6.03	118.38	111.02
1	A	50	HIS	O-C-N	6.02	130.28	122.87
1	F	229	ASP	CA-CB-CG	6.02	118.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	248	LYS	CB-CA-C	6.02	120.25	109.29
1	M	265	VAL	CB-CA-C	6.02	119.77	110.50
1	L	26	ASP	CA-CB-CG	-6.02	106.58	112.60
1	P	248	LYS	N-CA-C	-6.02	106.10	113.50
1	L	153	VAL	N-CA-CB	-6.01	101.31	111.23
1	M	39	ASP	CA-CB-CG	-6.01	106.59	112.60
1	M	265	VAL	N-CA-CB	-6.00	101.60	111.44
1	K	16	ALA	CA-C-O	-5.99	114.07	120.42
1	Q	51	GLN	CA-C-N	5.99	130.34	123.21
1	Q	51	GLN	C-N-CA	5.99	130.34	123.21
1	A	262	ARG	NE-CZ-NH2	5.98	124.58	119.20
1	D	198	ALA	CA-C-O	5.98	126.89	120.55
1	F	265	VAL	CB-CA-C	5.98	120.26	110.69
1	R	262	ARG	CB-CG-CD	5.98	125.05	111.30
1	T	126	CYS	CB-CA-C	5.97	120.71	110.79
1	M	233	LYS	N-CA-C	-5.97	104.85	111.36
1	I	52	GLN	CB-CA-C	-5.97	103.03	110.96
1	O	54	ARG	CD-NE-CZ	5.97	132.75	124.40
1	M	182	ILE	CB-CA-C	-5.96	101.80	110.63
1	O	248	LYS	N-CA-C	-5.95	106.18	113.50
1	G	217	SER	CA-C-O	-5.95	114.15	121.11
1	E	248	LYS	CA-C-O	5.95	125.68	119.14
1	T	159	ALA	CA-C-O	-5.93	114.13	120.42
1	R	51	GLN	CA-C-N	5.93	130.26	123.21
1	R	51	GLN	C-N-CA	5.93	130.26	123.21
1	C	182	ILE	CB-CA-C	-5.93	101.86	110.63
1	D	265	VAL	CB-CA-C	5.93	119.63	110.50
1	S	182	ILE	CB-CA-C	-5.93	102.00	110.83
1	D	126	CYS	CB-CA-C	5.92	120.62	110.79
1	D	248	LYS	CA-C-O	5.92	125.65	119.14
1	K	39	ASP	CA-CB-CG	-5.92	106.68	112.60
1	M	248	LYS	O-C-N	-5.92	114.56	122.49
1	D	199	GLN	CB-CG-CD	-5.91	102.55	112.60
1	L	164	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	T	39	ASP	CA-CB-CG	-5.91	106.69	112.60
1	T	123	LEU	CA-C-O	-5.91	114.29	120.55
1	H	265	VAL	N-CA-CB	-5.90	101.77	111.44
1	T	45	TYR	N-CA-C	5.90	119.78	112.59
1	F	164	GLN	CA-CB-CG	5.89	125.89	114.10
1	B	182	ILE	CB-CA-C	-5.89	102.05	110.83
1	H	126	CYS	CB-CA-C	5.89	120.57	110.79
1	K	145	THR	N-CA-C	5.89	118.21	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	163	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	A	45	TYR	N-CA-C	5.88	119.43	112.72
1	C	248	LYS	CA-C-O	5.88	125.61	119.14
1	S	248	LYS	CA-C-O	5.88	125.61	119.14
1	O	262	ARG	NH1-CZ-NH2	-5.88	111.66	119.30
1	O	182	ILE	CB-CA-C	-5.87	102.08	110.83
1	G	164	GLN	CG-CD-NE2	5.86	125.19	116.40
1	N	262	ARG	CA-C-O	-5.85	113.49	120.10
1	C	248	LYS	CB-CA-C	5.84	119.92	109.29
1	H	137	ARG	CD-NE-CZ	5.84	132.57	124.40
1	A	182	ILE	CB-CA-C	-5.83	102.00	110.63
1	E	16	ALA	CA-C-O	-5.83	114.70	120.70
1	A	159	ALA	CA-C-O	-5.82	114.70	120.70
1	R	265	VAL	CB-CA-C	5.82	119.47	110.50
1	P	39	ASP	CA-CB-CG	-5.82	106.78	112.60
1	J	233	LYS	N-CA-C	-5.81	105.03	111.36
1	A	60	GLN	OE1-CD-NE2	5.80	128.41	122.60
1	F	172	CYS	N-CA-C	5.80	118.35	111.33
1	A	248	LYS	CB-CA-C	5.80	119.85	109.29
1	P	265	VAL	CB-CA-C	5.80	119.43	110.50
1	H	137	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	K	195	GLN	OE1-CD-NE2	5.79	128.39	122.60
1	Q	266	THR	CA-C-O	5.79	124.92	119.59
1	R	262	ARG	CD-NE-CZ	5.78	132.50	124.40
1	H	248	LYS	CB-CA-C	5.78	119.80	109.29
1	A	262	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	P	265	VAL	N-CA-CB	-5.77	101.97	111.44
1	S	265	VAL	N-CA-CB	-5.77	101.97	111.44
1	J	249	GLN	N-CA-CB	5.77	121.29	111.66
1	F	31	GLY	CA-C-O	5.76	126.96	122.29
1	B	265	VAL	CB-CA-C	5.76	119.37	110.50
1	H	269	ALA	N-CA-C	5.76	118.02	111.11
1	K	70	PHE	CA-C-N	-5.75	116.06	123.19
1	K	70	PHE	C-N-CA	-5.75	116.06	123.19
1	M	49	PHE	CA-CB-CG	-5.75	108.05	113.80
1	N	182	ILE	N-CA-CB	5.75	119.07	111.25
1	I	217	SER	CA-C-O	-5.75	114.39	121.11
1	B	60	GLN	OE1-CD-NE2	5.74	128.34	122.60
1	N	163	ARG	NE-CZ-NH2	-5.74	114.03	119.20
1	A	265	VAL	CB-CA-C	5.74	119.33	110.50
1	N	156	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	D	156	ASN	OD1-CG-ND2	-5.73	116.87	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	126	CYS	CB-CA-C	5.73	120.30	110.79
1	I	262	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	K	97	SER	CA-CB-OG	-5.73	99.65	111.10
1	H	233	LYS	CA-C-O	5.72	126.48	120.42
1	L	49	PHE	CA-CB-CG	-5.72	108.08	113.80
1	Q	198	ALA	CA-C-O	5.72	126.61	120.55
1	G	182	ILE	N-CA-CB	5.71	119.02	111.25
1	J	248	LYS	CB-CA-C	5.71	119.69	109.29
1	K	207	VAL	CA-C-O	-5.71	114.47	120.76
1	T	145	THR	N-CA-C	5.71	117.98	111.02
1	A	266	THR	CA-C-O	5.71	124.84	119.59
1	D	164	GLN	CA-CB-CG	5.71	125.51	114.10
1	T	221	LEU	N-CA-CB	-5.71	101.74	110.01
1	G	243	SER	O-C-N	-5.70	114.79	122.43
1	T	163	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	E	145	THR	N-CA-C	5.70	117.97	111.02
1	D	137	ARG	CD-NE-CZ	5.69	132.37	124.40
1	K	153	VAL	N-CA-CB	-5.69	101.84	111.23
1	Q	126	CYS	O-C-N	-5.69	116.09	122.12
1	H	159	ALA	O-C-N	5.69	128.23	122.09
1	Q	28	ARG	CB-CA-C	-5.69	110.00	116.54
1	D	145	THR	N-CA-C	5.68	117.95	111.02
1	B	145	THR	N-CA-C	5.67	117.94	111.02
1	D	248	LYS	N-CA-C	-5.67	106.52	113.50
1	Q	160	VAL	N-CA-CB	5.67	120.03	110.56
1	I	176	PHE	CA-CB-CG	5.67	119.47	113.80
1	G	145	THR	N-CA-C	5.67	117.94	111.02
1	R	182	ILE	N-CA-CB	5.67	119.23	111.41
1	Q	145	THR	N-CA-C	5.66	117.93	111.02
1	B	182	ILE	N-CA-CB	5.66	118.95	111.25
1	Q	265	VAL	N-CA-CB	-5.66	101.46	111.93
1	S	262	ARG	NH1-CZ-NH2	-5.66	111.94	119.30
1	B	39	ASP	CA-CB-CG	-5.65	106.95	112.60
1	N	126	CYS	N-CA-CB	-5.65	101.81	110.12
1	A	171	GLU	CB-CG-CD	5.65	122.21	112.60
1	L	126	CYS	CB-CA-C	5.65	120.17	110.79
1	M	182	ILE	N-CA-CB	5.65	119.20	111.41
1	E	248	LYS	CB-CA-C	5.65	119.56	109.29
1	R	248	LYS	CB-CA-C	5.64	119.56	109.29
1	P	126	CYS	CB-CA-C	5.64	120.16	110.79
1	C	126	CYS	CB-CA-C	5.64	120.15	110.79
1	F	248	LYS	CB-CA-C	5.64	119.55	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	49	PHE	CA-CB-CG	-5.63	108.17	113.80
1	H	248	LYS	N-CA-C	-5.62	106.59	113.50
1	O	126	CYS	N-CA-CB	-5.62	101.86	110.01
1	F	221	LEU	O-C-N	-5.61	116.25	122.09
1	I	249	GLN	N-CA-CB	5.61	121.02	111.66
1	G	164	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	R	23	LYS	O-C-N	-5.60	114.93	122.43
1	C	265	VAL	CB-CA-C	5.60	119.64	110.69
1	I	182	ILE	N-CA-CB	5.59	119.13	111.41
1	C	45	TYR	N-CA-C	5.59	119.41	112.59
1	G	24	GLY	N-CA-C	-5.59	107.05	115.32
1	N	126	CYS	CB-CA-C	5.59	120.07	110.79
1	B	265	VAL	N-CA-CB	-5.59	102.28	111.44
1	S	70	PHE	CA-C-O	-5.59	114.58	121.06
1	B	209	TRP	CA-C-O	-5.58	114.62	120.09
1	L	198	ALA	CA-C-O	5.58	126.47	120.55
1	O	52	GLN	OE1-CD-NE2	-5.58	117.02	122.60
1	T	153	VAL	N-CA-CB	-5.57	102.04	111.23
1	T	195	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	K	66	ALA	N-CA-CB	-5.57	101.86	110.04
1	F	83	GLN	OE1-CD-NE2	5.56	128.16	122.60
1	L	54	ARG	CD-NE-CZ	5.56	132.19	124.40
1	R	50	HIS	CA-CB-CG	5.56	119.36	113.80
1	H	181	GLY	CA-C-O	-5.56	116.53	121.64
1	I	91	GLY	CA-C-N	-5.56	115.89	123.12
1	I	91	GLY	C-N-CA	-5.56	115.89	123.12
1	F	36	ARG	CA-C-O	-5.56	114.72	121.05
1	N	262	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	T	163	ARG	N-CA-CB	5.56	118.39	110.16
1	G	147	LEU	O-C-N	-5.55	116.35	122.07
1	B	172	CYS	N-CA-C	5.54	118.04	111.33
1	C	163	ARG	NE-CZ-NH1	5.54	127.04	121.50
1	R	38	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	262	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	K	176	PHE	CA-CB-CG	5.53	119.33	113.80
1	Q	262	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	R	128	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	K	159	ALA	CA-C-O	-5.53	114.56	120.42
1	B	262	ARG	CD-NE-CZ	5.53	132.14	124.40
1	F	145	THR	N-CA-C	5.53	117.76	111.02
1	T	248	LYS	CA-C-O	5.53	125.22	119.14
1	K	26	ASP	CA-CB-CG	-5.52	107.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	52	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	I	145	THR	N-CA-C	5.52	117.75	111.02
1	E	137	ARG	NE-CZ-NH2	5.52	124.17	119.20
1	A	221	LEU	O-C-N	-5.51	116.39	122.07
1	N	164	GLN	CA-CB-CG	5.51	125.12	114.10
1	N	199	GLN	N-CA-CB	-5.50	102.01	110.16
1	B	38	ASP	CA-CB-CG	5.49	118.09	112.60
1	D	262	ARG	CB-CG-CD	5.49	123.93	111.30
1	F	262	ARG	NE-CZ-NH2	5.49	124.14	119.20
1	I	223	GLU	CG-CD-OE2	-5.49	105.78	118.40
1	N	265	VAL	CB-CA-C	5.49	119.47	110.69
1	J	176	PHE	CA-CB-CG	5.48	119.28	113.80
1	D	171	GLU	CB-CG-CD	5.48	121.92	112.60
1	R	176	PHE	CA-CB-CG	5.48	119.28	113.80
1	T	164	GLN	CA-CB-CG	5.48	125.06	114.10
1	S	51	GLN	N-CA-C	5.48	117.25	111.28
1	L	38	ASP	CA-C-O	-5.47	115.22	121.68
1	L	137	ARG	NE-CZ-NH2	5.47	124.13	119.20
1	O	36	ARG	CA-C-O	-5.47	114.81	121.05
1	L	126	CYS	N-CA-CB	-5.46	102.09	110.12
1	C	164	GLN	CA-CB-CG	5.46	125.02	114.10
1	N	248	LYS	CB-CA-C	5.46	119.23	109.29
1	O	245	GLY	CA-C-O	-5.46	112.81	119.03
1	A	16	ALA	CA-C-O	-5.46	115.08	120.70
1	O	70	PHE	CA-C-N	-5.46	116.42	123.19
1	O	70	PHE	C-N-CA	-5.46	116.42	123.19
1	P	172	CYS	N-CA-C	5.46	117.23	111.28
1	A	198	ALA	O-C-N	-5.46	116.34	122.12
1	B	137	ARG	CD-NE-CZ	5.45	132.04	124.40
1	C	265	VAL	N-CA-CB	-5.45	101.85	111.93
1	H	262	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	I	49	PHE	CA-CB-CG	-5.44	108.36	113.80
1	G	126	CYS	CB-CA-C	5.44	119.82	110.79
1	G	248	LYS	CA-C-O	5.44	125.12	119.14
1	S	145	THR	N-CA-C	5.44	117.66	111.02
1	S	248	LYS	CB-CA-C	5.44	119.19	109.29
1	A	209	TRP	CA-C-O	-5.44	114.76	120.09
1	Q	248	LYS	O-C-N	-5.44	115.20	122.49
1	B	229	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	223	GLU	CG-CD-OE2	-5.44	105.90	118.40
1	F	269	ALA	N-CA-C	5.43	116.88	111.07
1	B	153	VAL	N-CA-CB	-5.43	102.28	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	52	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	J	223	GLU	CG-CD-OE2	-5.42	105.93	118.40
1	N	248	LYS	N-CA-C	-5.42	106.83	113.50
1	G	221	LEU	O-C-N	-5.42	116.45	122.09
1	D	249	GLN	N-CA-CB	5.42	120.71	111.66
1	B	248	LYS	N-CA-C	-5.42	106.84	113.50
1	F	196	ALA	O-C-N	5.42	127.86	122.12
1	C	38	ASP	CA-CB-CG	5.41	118.01	112.60
1	O	221	LEU	O-C-N	-5.41	116.46	122.09
1	C	221	LEU	O-C-N	-5.41	116.46	122.09
1	E	265	VAL	CB-CA-C	5.41	118.83	110.50
1	P	262	ARG	NE-CZ-NH2	5.41	124.07	119.20
1	N	198	ALA	CA-C-O	5.40	126.28	120.55
1	N	45	TYR	N-CA-C	5.39	119.17	112.59
1	N	215	PHE	CA-C-N	-5.39	116.34	121.46
1	N	215	PHE	C-N-CA	-5.39	116.34	121.46
1	H	28	ARG	CD-NE-CZ	5.39	131.95	124.40
1	S	143	HIS	CA-CB-CG	-5.39	108.41	113.80
1	T	171	GLU	CB-CG-CD	5.39	121.76	112.60
1	O	133	ASN	CA-CB-CG	-5.39	107.21	112.60
1	C	193	ILE	CA-C-N	5.39	125.92	119.94
1	C	193	ILE	C-N-CA	5.39	125.92	119.94
1	H	217	SER	CA-C-O	-5.39	114.81	121.11
1	K	70	PHE	CA-CB-CG	5.39	119.19	113.80
1	E	266	THR	CA-C-O	5.38	124.54	119.59
1	B	126	CYS	CB-CA-C	5.38	119.72	110.79
1	D	153	VAL	N-CA-CB	-5.38	102.35	111.23
1	E	60	GLN	OE1-CD-NE2	5.38	127.98	122.60
1	D	160	VAL	N-CA-CB	5.37	118.64	110.58
1	J	265	VAL	CB-CA-C	5.37	118.77	110.50
1	O	163	ARG	CA-C-O	-5.37	114.73	120.42
1	H	182	ILE	N-CA-CB	5.37	118.55	111.25
1	T	248	LYS	CB-CA-C	5.37	119.06	109.29
1	F	126	CYS	CB-CA-C	5.37	119.69	110.79
1	H	262	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	I	51	GLN	N-CA-C	5.36	117.13	111.28
1	D	233	LYS	N-CA-C	-5.36	105.52	111.36
1	I	265	VAL	CB-CA-C	5.36	119.27	110.69
1	L	262	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	T	199	GLN	CB-CG-CD	-5.36	103.49	112.60
1	T	249	GLN	N-CA-CB	5.36	120.61	111.66
1	P	248	LYS	CA-C-O	5.36	125.03	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	223	GLU	CG-CD-OE2	-5.36	106.08	118.40
1	I	143	HIS	CA-CB-CG	-5.35	108.45	113.80
1	Q	153	VAL	N-CA-CB	-5.34	102.41	111.23
1	I	32	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	L	249	GLN	N-CA-CB	5.34	120.58	111.66
1	H	182	ILE	CB-CA-C	-5.34	102.88	110.83
1	L	9	PHE	CA-C-N	-5.34	112.84	120.42
1	L	9	PHE	C-N-CA	-5.34	112.84	120.42
1	F	223	GLU	CG-CD-OE2	-5.34	106.13	118.40
1	B	221	LEU	N-CA-CB	-5.33	102.27	110.01
1	Q	45	TYR	N-CA-C	5.33	119.10	112.59
1	R	156	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	R	215	PHE	CA-C-O	-5.33	114.53	120.66
1	H	198	ALA	CA-C-O	5.33	126.20	120.55
1	T	199	GLN	N-CA-CB	-5.33	102.28	110.01
1	E	265	VAL	N-CA-CB	-5.33	102.70	111.44
1	M	223	GLU	CG-CD-OE2	-5.33	106.14	118.40
1	G	181	GLY	CA-C-O	-5.33	116.74	121.64
1	J	164	GLN	CG-CD-NE2	5.33	124.39	116.40
1	H	60	GLN	CA-C-O	5.32	124.45	119.13
1	B	42	ILE	O-C-N	-5.32	116.89	122.20
1	L	182	ILE	CB-CA-C	-5.32	102.91	110.83
1	K	184	PRO	N-CA-C	-5.31	103.44	111.41
1	I	163	ARG	NE-CZ-NH2	-5.31	114.42	119.20
1	I	253	ARG	NE-CZ-NH1	5.31	126.81	121.50
1	C	182	ILE	N-CA-CB	5.31	118.73	111.41
1	T	246	GLY	O-C-N	-5.31	116.89	123.21
1	R	233	LYS	CA-C-O	5.30	126.04	120.42
1	F	202	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	N	49	PHE	CA-CB-CG	-5.30	108.50	113.80
1	O	176	PHE	CA-CB-CG	5.30	119.10	113.80
1	O	248	LYS	CA-C-O	5.30	124.97	119.14
1	M	164	GLN	CA-CB-CG	5.29	124.69	114.10
1	F	60	GLN	OE1-CD-NE2	5.29	127.89	122.60
1	B	223	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	I	81	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	P	221	LEU	O-C-N	-5.29	116.59	122.09
1	K	9	PHE	CA-C-O	-5.28	114.38	120.24
1	D	266	THR	CA-C-N	5.28	125.19	119.76
1	D	266	THR	C-N-CA	5.28	125.19	119.76
1	M	125	HIS	CA-C-O	5.28	126.36	120.82
1	T	182	ILE	N-CA-CB	5.28	118.42	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	182	ILE	N-CA-CB	5.27	118.42	111.25
1	T	126	CYS	N-CA-CB	-5.27	102.37	110.12
1	H	164	GLN	CA-CB-CG	5.27	124.65	114.10
1	L	221	LEU	O-C-N	-5.27	116.53	122.12
1	P	128	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	D	51	GLN	CA-C-N	5.27	129.48	123.21
1	D	51	GLN	C-N-CA	5.27	129.48	123.21
1	H	195	GLN	CB-CG-CD	-5.26	103.65	112.60
1	K	148	ILE	O-C-N	-5.26	116.75	121.91
1	Q	164	GLN	CA-CB-CG	5.26	124.63	114.10
1	R	249	GLN	N-CA-CB	5.26	120.45	111.66
1	L	123	LEU	CA-C-O	-5.25	114.98	120.55
1	B	223	GLU	OE1-CD-OE2	5.25	135.51	122.90
1	H	195	GLN	O-C-N	5.25	127.48	122.07
1	O	164	GLN	OE1-CD-NE2	-5.25	117.35	122.60
1	S	172	CYS	N-CA-C	5.25	117.00	111.28
1	F	172	CYS	CA-C-N	5.25	127.31	120.28
1	F	172	CYS	C-N-CA	5.25	127.31	120.28
1	P	179	GLY	CA-C-N	-5.25	116.27	123.14
1	P	179	GLY	C-N-CA	-5.25	116.27	123.14
1	P	215	PHE	CA-C-N	-5.25	117.07	121.58
1	P	215	PHE	C-N-CA	-5.25	117.07	121.58
1	E	262	ARG	CD-NE-CZ	5.24	131.74	124.40
1	I	221	LEU	O-C-N	-5.24	116.64	122.09
1	L	262	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	O	9	PHE	CA-C-N	-5.24	112.97	120.42
1	O	9	PHE	C-N-CA	-5.24	112.97	120.42
1	B	163	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	D	159	ALA	CA-C-O	-5.24	114.87	120.42
1	K	265	VAL	CB-CA-C	5.23	118.56	110.50
1	G	83	GLN	OE1-CD-NE2	5.23	127.83	122.60
1	I	198	ALA	CA-C-O	5.23	126.09	120.55
1	A	137	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	L	221	LEU	N-CA-CB	-5.22	102.44	110.12
1	M	185	TRP	CA-C-O	-5.22	115.45	121.19
1	A	258	ALA	CA-C-N	5.22	127.23	120.44
1	A	258	ALA	C-N-CA	5.22	127.23	120.44
1	D	262	ARG	CD-NE-CZ	5.22	131.71	124.40
1	E	223	GLU	CG-CD-OE2	-5.22	106.40	118.40
1	G	153	VAL	N-CA-CB	-5.21	102.62	111.23
1	T	182	ILE	CB-CA-C	-5.21	103.06	110.83
1	D	163	ARG	NE-CZ-NH1	5.21	126.71	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	265	VAL	N-CA-CB	-5.21	102.90	111.44
1	Q	217	SER	CA-C-O	-5.21	115.02	121.11
1	D	181	GLY	CA-C-O	-5.21	116.85	121.64
1	C	248	LYS	O-C-N	-5.21	115.52	122.49
1	C	253	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	K	143	HIS	CE1-NE2-CD2	5.20	114.20	109.00
1	J	243	SER	N-CA-C	-5.20	106.19	112.54
1	R	168	GLY	N-CA-C	5.20	120.39	114.67
1	F	39	ASP	CA-CB-CG	-5.20	107.40	112.60
1	N	253	ARG	NE-CZ-NH1	5.20	126.70	121.50
1	O	137	ARG	CD-NE-CZ	5.20	131.68	124.40
1	O	198	ALA	CA-C-O	5.20	125.97	120.10
1	A	223	GLU	OE1-CD-OE2	5.20	135.37	122.90
1	C	11	GLN	OE1-CD-NE2	-5.19	117.41	122.60
1	P	182	ILE	N-CA-CB	5.19	118.31	111.25
1	K	262	ARG	NH1-CZ-NH2	-5.19	112.55	119.30
1	F	233	LYS	CA-C-O	5.18	125.91	120.42
1	H	221	LEU	N-CA-CB	-5.18	102.50	110.01
1	O	262	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	M	143	HIS	CA-CB-CG	-5.17	108.63	113.80
1	D	182	ILE	CB-CA-C	-5.17	103.13	110.83
1	J	262	ARG	NE-CZ-NH1	5.17	126.67	121.50
1	N	248	LYS	CA-C-O	5.17	124.83	119.14
1	D	272	LEU	N-CA-C	-5.17	105.72	112.23
1	T	70	PHE	CA-C-N	-5.17	116.78	123.19
1	T	70	PHE	C-N-CA	-5.17	116.78	123.19
1	N	163	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	O	146	ASN	CA-CB-CG	-5.16	107.44	112.60
1	F	163	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	F	265	VAL	N-CA-CB	-5.16	102.38	111.93
1	N	134	GLY	CA-C-O	-5.16	112.64	119.25
1	S	233	LYS	N-CA-C	-5.16	105.73	111.36
1	Q	163	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	M	270	SER	CA-C-O	-5.15	115.09	120.55
1	B	221	LEU	O-C-N	-5.15	116.77	122.07
1	R	39	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	80	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	I	147	LEU	CA-C-O	-5.15	115.09	120.55
1	N	145	THR	N-CA-C	5.14	117.29	111.02
1	K	170	THR	CA-CB-OG1	-5.14	101.90	109.60
1	R	248	LYS	CA-C-O	5.14	124.79	119.14
1	S	248	LYS	O-C-N	-5.14	115.61	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	38	ASP	CA-CB-CG	5.13	117.73	112.60
1	O	181	GLY	CA-C-O	-5.13	116.66	121.18
1	Q	248	LYS	CA-C-N	5.13	130.29	121.87
1	Q	248	LYS	C-N-CA	5.13	130.29	121.87
1	T	262	ARG	CA-C-O	-5.13	114.30	120.10
1	B	159	ALA	CA-C-O	-5.13	115.42	120.70
1	H	60	GLN	CG-CD-NE2	5.13	124.09	116.40
1	J	182	ILE	N-CA-CB	5.13	118.49	111.41
1	P	248	LYS	CB-CA-C	5.13	118.63	109.29
1	Q	223	GLU	CG-CD-OE2	-5.13	106.60	118.40
1	C	229	ASP	CA-CB-CG	5.13	117.73	112.60
1	F	5	THR	CA-C-O	-5.13	113.29	119.49
1	T	221	LEU	O-C-N	-5.13	116.79	122.07
1	I	160	VAL	N-CA-CB	5.12	118.27	110.58
1	O	223	GLU	CG-CD-OE2	-5.12	106.62	118.40
1	P	123	LEU	CA-C-O	-5.12	115.12	120.55
1	F	185	TRP	CA-C-O	-5.12	115.56	121.19
1	G	215	PHE	CA-C-O	-5.12	114.77	120.66
1	J	126	CYS	N-CA-CB	-5.12	102.60	110.12
1	P	125	HIS	CA-C-O	5.12	126.19	120.82
1	B	81	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	164	GLN	CA-CB-CG	5.11	124.33	114.10
1	G	26	ASP	CA-CB-CG	-5.11	107.49	112.60
1	H	126	CYS	O-C-N	-5.11	116.70	122.12
1	K	98	ASP	CA-CB-CG	-5.11	107.49	112.60
1	Q	193	ILE	CA-C-N	5.11	125.61	119.94
1	Q	193	ILE	C-N-CA	5.11	125.61	119.94
1	S	23	LYS	O-C-N	-5.11	115.58	122.43
1	D	223	GLU	OE1-CD-OE2	5.10	135.15	122.90
1	F	182	ILE	CB-CA-C	-5.10	103.08	110.63
1	I	38	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	172	CYS	N-CA-C	5.10	116.84	111.28
1	H	171	GLU	CB-CG-CD	5.10	121.27	112.60
1	G	148	ILE	O-C-N	-5.10	116.92	121.91
1	O	26	ASP	CA-CB-CG	-5.10	107.50	112.60
1	D	182	ILE	N-CA-CB	5.09	118.17	111.25
1	M	266	THR	CA-C-O	5.09	124.42	119.99
1	G	249	GLN	N-CA-CB	5.08	120.15	111.66
1	D	241	VAL	N-CA-C	5.08	115.30	110.42
1	H	229	ASP	CA-CB-CG	5.08	117.68	112.60
1	L	199	GLN	N-CA-CB	-5.08	102.64	110.01
1	O	83	GLN	OE1-CD-NE2	5.08	127.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	70	PHE	CA-C-N	-5.08	116.89	123.19
1	J	70	PHE	C-N-CA	-5.08	116.89	123.19
1	R	97	SER	CA-C-O	-5.08	114.36	120.10
1	Q	182	ILE	N-CA-CB	5.07	118.41	111.41
1	K	215	PHE	CA-C-N	-5.07	116.13	121.35
1	K	215	PHE	C-N-CA	-5.07	116.13	121.35
1	K	262	ARG	CD-NE-CZ	5.07	131.50	124.40
1	H	126	CYS	N-CA-CB	-5.07	102.67	110.12
1	A	261	LYS	CA-C-O	-5.07	115.50	120.82
1	D	50	HIS	CA-CB-CG	5.07	118.87	113.80
1	E	172	CYS	N-CA-C	5.07	117.46	111.33
1	P	223	GLU	CA-C-O	-5.07	115.05	120.42
1	G	54	ARG	CD-NE-CZ	5.07	131.49	124.40
1	P	249	GLN	N-CA-CB	5.07	120.12	111.66
1	S	229	ASP	CA-CB-CG	5.07	117.67	112.60
1	G	262	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	Q	50	HIS	N-CA-C	-5.06	103.47	110.35
1	M	95	VAL	CA-C-O	-5.05	115.82	121.23
1	T	265	VAL	N-CA-CB	-5.05	103.16	111.44
1	C	153	VAL	N-CA-CB	-5.05	102.90	111.23
1	H	45	TYR	N-CA-C	5.05	118.75	112.59
1	I	209	TRP	CA-C-O	-5.05	115.14	120.09
1	K	126	CYS	CB-CA-C	5.05	119.26	110.68
1	T	50	HIS	CA-CB-CG	5.04	118.84	113.80
1	K	223	GLU	O-C-N	5.04	128.47	122.27
1	H	39	ASP	CA-CB-CG	-5.04	107.56	112.60
1	P	67	ASN	CA-CB-CG	-5.04	107.56	112.60
1	P	223	GLU	CG-CD-OE2	-5.04	106.80	118.40
1	A	123	LEU	CA-C-O	-5.04	115.21	120.55
1	I	265	VAL	N-CA-CB	-5.04	102.61	111.93
1	E	182	ILE	N-CA-CB	5.04	118.36	111.41
1	N	146	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	T	253	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	S	137	ARG	CD-NE-CZ	5.03	131.45	124.40
1	A	51	GLN	N-CA-C	5.03	116.76	111.28
1	E	221	LEU	O-C-N	-5.03	116.89	122.07
1	F	126	CYS	N-CA-CB	-5.03	102.73	110.12
1	C	262	ARG	CD-NE-CZ	5.02	131.43	124.40
1	M	229	ASP	CA-CB-CG	5.02	117.62	112.60
1	O	153	VAL	N-CA-CB	-5.02	102.95	111.23
1	A	95	VAL	CA-C-O	-5.02	115.86	121.23
1	P	126	CYS	N-CA-CB	-5.01	102.75	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	70	PHE	CA-C-N	-5.01	116.97	123.19
1	S	70	PHE	C-N-CA	-5.01	116.97	123.19
1	R	265	VAL	N-CA-CB	-5.01	103.22	111.44
1	G	198	ALA	O-C-N	-5.01	116.81	122.12
1	G	265	VAL	CB-CA-C	5.01	118.22	110.50
1	R	45	TYR	N-CA-C	5.01	118.70	112.59
1	S	221	LEU	N-CA-CB	-5.01	102.75	110.01
1	E	54	ARG	CD-NE-CZ	5.01	131.41	124.40
1	K	15	LYS	CA-C-O	5.01	126.08	120.82
1	H	62	MET	CA-C-N	5.00	124.78	119.28
1	H	62	MET	C-N-CA	5.00	124.78	119.28
1	P	38	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	38	ASP	Mainchain
1	F	38	ASP	Mainchain
1	I	38	ASP	Mainchain
1	L	38	ASP	Mainchain
1	N	38	ASP	Mainchain
1	P	38	ASP	Mainchain
1	Q	38	ASP	Mainchain

5.2 Too-close contacts [i](#)

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	2124	0	2097	44	0
1	B	2124	0	2097	37	0
1	C	2124	0	2097	37	0
1	D	2124	0	2097	40	2
1	E	2124	0	2097	36	1
1	F	2124	0	2097	31	0
1	G	2124	0	2097	40	0
1	H	2124	0	2097	43	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2124	0	2097	42	0
1	J	2124	0	2097	43	0
1	K	2124	0	2097	45	8
1	L	2124	0	2097	37	2
1	M	2124	0	2097	46	2
1	N	2124	0	2097	42	0
1	O	2124	0	2097	42	0
1	P	2124	0	2097	40	0
1	Q	2124	0	2097	36	0
1	R	2124	0	2097	34	0
1	S	2124	0	2097	36	9
1	T	2124	0	2097	48	3
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	S	1	0	0	0	0
2	T	1	0	0	0	0
3	A	10	0	3	0	0
3	B	10	0	3	0	0
3	C	10	0	3	0	0
3	D	10	0	3	0	0
3	E	10	0	3	0	0
3	F	10	0	3	0	0
3	G	10	0	3	0	0
3	H	10	0	3	1	0
3	I	10	0	3	0	0
3	J	10	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	10	0	3	0	0
3	L	10	0	3	0	0
3	M	10	0	3	0	0
3	N	10	0	3	0	0
3	O	10	0	3	0	0
3	P	10	0	3	0	0
3	Q	10	0	3	0	0
3	R	10	0	3	0	0
3	S	10	0	3	0	0
3	T	10	0	3	0	0
4	A	177	0	0	17	0
4	B	174	0	0	16	0
4	C	173	0	0	14	0
4	D	173	0	0	21	0
4	E	179	0	0	16	0
4	F	174	0	0	14	0
4	G	176	0	0	14	0
4	H	171	0	0	19	2
4	I	177	0	0	16	0
4	J	178	0	0	16	0
4	K	177	0	0	22	1
4	L	167	0	0	13	0
4	M	183	0	0	18	0
4	N	170	0	0	16	0
4	O	175	0	0	15	0
4	P	167	0	0	19	0
4	Q	176	0	0	16	0
4	R	172	0	0	14	1
4	S	171	0	0	17	0
4	T	170	0	0	26	0
All	All	46180	0	42000	786	17

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 9.

All (786) 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:K:97:SER:CB	4:K:2077:HOH:O	1.66	1.28
1:T:157:ASP:CG	4:T:2105:HOH:O	1.83	1.20
1:K:97:SER:HB3	4:K:2077:HOH:O	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:163:ARG:NH2	1:P:274:LEU:OXT	1.91	1.03
1:K:163:ARG:NH2	1:K:274:LEU:OXT	1.93	1.02
1:H:127:GLU:OE2	4:H:2099:HOH:O	1.77	1.01
1:J:163:ARG:NH2	1:J:274:LEU:OXT	1.94	1.01
1:D:46:HIS:HB2	4:D:2054:HOH:O	1.61	1.00
1:N:163:ARG:NH2	1:N:274:LEU:OXT	1.95	1.00
1:T:157:ASP:HA	4:T:2104:HOH:O	1.62	1.00
1:O:46:HIS:HB2	4:O:2058:HOH:O	1.61	0.99
1:F:163:ARG:NH2	1:F:274:LEU:OXT	1.96	0.99
1:O:163:ARG:NH2	1:O:274:LEU:OXT	1.96	0.99
1:E:163:ARG:NH2	1:E:274:LEU:OXT	1.96	0.98
1:I:163:ARG:NH2	1:I:274:LEU:OXT	1.96	0.97
1:H:163:ARG:NH2	1:H:274:LEU:OXT	1.98	0.97
1:L:163:ARG:NH2	1:L:274:LEU:OXT	1.98	0.96
1:Q:163:ARG:NH2	1:Q:274:LEU:OXT	2.00	0.95
1:G:163:ARG:NH2	1:G:274:LEU:OXT	1.99	0.94
1:K:97:SER:CA	4:K:2077:HOH:O	1.97	0.94
1:R:163:ARG:NH2	1:R:274:LEU:OXT	2.01	0.94
1:A:163:ARG:NH2	1:A:274:LEU:OXT	2.01	0.93
1:Q:46:HIS:HB2	4:Q:2064:HOH:O	1.67	0.93
1:N:46:HIS:HB2	4:N:2056:HOH:O	1.67	0.93
1:T:157:ASP:OD2	4:T:2105:HOH:O	1.78	0.93
1:T:157:ASP:CA	4:T:2104:HOH:O	2.18	0.92
1:G:46:HIS:HB2	4:G:2061:HOH:O	1.70	0.91
1:T:157:ASP:OD1	4:T:2105:HOH:O	1.78	0.91
1:B:163:ARG:NH2	1:B:274:LEU:OXT	2.03	0.91
1:M:163:ARG:NH2	1:M:274:LEU:OXT	2.04	0.90
1:T:46:HIS:HB2	4:T:2055:HOH:O	1.70	0.90
1:H:46:HIS:HB2	4:H:2057:HOH:O	1.72	0.90
1:C:163:ARG:NH2	1:C:274:LEU:OXT	2.05	0.90
1:T:163:ARG:NH2	1:T:274:LEU:OXT	2.03	0.89
1:T:157:ASP:CB	4:T:2104:HOH:O	2.20	0.89
1:K:97:SER:O	4:K:2095:HOH:O	1.65	0.89
1:I:91:GLY:HA3	1:I:108:LEU:HD22	1.55	0.89
1:S:163:ARG:NH2	1:S:274:LEU:OXT	2.04	0.89
1:O:91:GLY:HA3	1:O:108:LEU:HD22	1.56	0.88
1:L:91:GLY:HA3	1:L:108:LEU:HD22	1.56	0.88
1:F:46:HIS:HB2	4:F:2059:HOH:O	1.74	0.87
1:D:163:ARG:NH2	1:D:274:LEU:OXT	2.07	0.87
1:M:46:HIS:HB2	4:M:2066:HOH:O	1.74	0.86
1:P:46:HIS:HB2	4:P:2049:HOH:O	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:91:GLY:HA3	1:Q:108:LEU:HD22	1.58	0.85
1:K:91:GLY:HA3	1:K:108:LEU:HD22	1.56	0.85
1:N:91:GLY:HA3	1:N:108:LEU:HD22	1.60	0.84
1:N:248:LYS:NZ	4:N:2155:HOH:O	2.10	0.84
1:P:91:GLY:HA3	1:P:108:LEU:HD22	1.58	0.84
1:O:46:HIS:HE1	4:O:2059:HOH:O	1.61	0.84
1:E:46:HIS:HB2	4:E:2067:HOH:O	1.78	0.84
1:G:91:GLY:HA3	1:G:108:LEU:HD22	1.59	0.83
1:T:157:ASP:OD2	4:T:2104:HOH:O	1.93	0.83
1:K:46:HIS:HB2	4:K:2062:HOH:O	1.79	0.83
1:J:91:GLY:HA3	1:J:108:LEU:HD22	1.61	0.82
1:B:91:GLY:HA3	1:B:108:LEU:HD22	1.60	0.82
1:C:46:HIS:HB2	4:C:2061:HOH:O	1.80	0.81
1:F:91:GLY:HA3	1:F:108:LEU:HD22	1.60	0.81
1:T:91:GLY:HA3	1:T:108:LEU:HD22	1.63	0.81
1:C:91:GLY:HA3	1:C:108:LEU:HD22	1.62	0.81
1:G:178:ASP:O	1:G:204:HIS:HD2	1.64	0.80
1:D:91:GLY:HA3	1:D:108:LEU:HD22	1.62	0.80
1:K:97:SER:HA	4:K:2077:HOH:O	1.67	0.80
1:M:28:ARG:HD2	4:M:2043:HOH:O	1.80	0.80
1:M:91:GLY:HA3	1:M:108:LEU:HD22	1.63	0.80
1:J:28:ARG:HD2	4:J:2039:HOH:O	1.80	0.80
1:R:91:GLY:HA3	1:R:108:LEU:HD22	1.63	0.80
1:A:91:GLY:HA3	1:A:108:LEU:HD22	1.64	0.80
1:H:91:GLY:HA3	1:H:108:LEU:HD22	1.64	0.80
1:Q:46:HIS:HE1	4:Q:2065:HOH:O	1.64	0.80
1:I:46:HIS:HB2	4:I:2064:HOH:O	1.80	0.80
1:Q:243:SER:O	4:Q:2160:HOH:O	2.00	0.79
1:A:46:HIS:HB2	4:A:2066:HOH:O	1.82	0.79
1:K:243:SER:O	4:K:2157:HOH:O	1.98	0.79
1:D:243:SER:O	4:D:2152:HOH:O	1.99	0.79
1:H:243:SER:O	4:H:2152:HOH:O	1.99	0.79
1:L:46:HIS:HB2	4:L:2055:HOH:O	1.82	0.79
1:O:248:LYS:NZ	4:O:2160:HOH:O	2.16	0.78
1:E:91:GLY:HA3	1:E:108:LEU:HD22	1.63	0.78
1:O:178:ASP:O	1:O:204:HIS:HD2	1.67	0.78
1:D:147:LEU:HD13	1:D:235:ALA:HB2	1.66	0.77
1:B:46:HIS:HB2	4:B:2062:HOH:O	1.83	0.77
1:D:46:HIS:HE1	4:D:2055:HOH:O	1.67	0.77
1:H:28:ARG:HD2	4:H:2037:HOH:O	1.85	0.77
1:L:147:LEU:HD13	1:L:235:ALA:HB2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:46:HIS:HB2	4:R:2060:HOH:O	1.84	0.77
1:G:147:LEU:HD13	1:G:235:ALA:HB2	1.67	0.77
1:K:178:ASP:O	1:K:204:HIS:HD2	1.67	0.77
1:P:147:LEU:HD13	1:P:235:ALA:HB2	1.66	0.76
1:A:178:ASP:O	1:A:204:HIS:HD2	1.68	0.76
1:N:243:SER:O	4:N:2150:HOH:O	2.04	0.76
1:F:243:SER:O	4:F:2154:HOH:O	2.03	0.76
1:L:28:ARG:HD2	4:L:2034:HOH:O	1.86	0.76
1:P:243:SER:O	4:P:2147:HOH:O	2.03	0.75
1:T:243:SER:O	4:T:2150:HOH:O	2.03	0.75
1:A:147:LEU:HD13	1:A:235:ALA:HB2	1.68	0.75
1:Q:164:GLN:NE2	4:Q:2120:HOH:O	2.18	0.75
1:S:46:HIS:HB2	4:S:2059:HOH:O	1.85	0.75
1:F:178:ASP:O	1:F:204:HIS:HD2	1.70	0.75
1:L:243:SER:O	4:L:2147:HOH:O	2.04	0.75
1:D:178:ASP:O	1:D:204:HIS:HD2	1.70	0.75
1:D:248:LYS:NZ	4:D:2157:HOH:O	2.19	0.75
1:M:147:LEU:HD13	1:M:235:ALA:HB2	1.67	0.75
1:P:178:ASP:O	1:P:204:HIS:HD2	1.70	0.75
1:S:147:LEU:HD13	1:S:235:ALA:HB2	1.67	0.75
1:B:113:VAL:HG11	1:I:57:PRO:HD3	1.69	0.74
1:L:178:ASP:O	1:L:204:HIS:HD2	1.70	0.74
1:S:91:GLY:HA3	1:S:108:LEU:HD22	1.68	0.74
1:E:178:ASP:O	1:E:204:HIS:HD2	1.70	0.74
1:I:147:LEU:HD13	1:I:235:ALA:HB2	1.68	0.74
1:O:147:LEU:HD13	1:O:235:ALA:HB2	1.70	0.74
1:H:147:LEU:HD13	1:H:235:ALA:HB2	1.70	0.74
1:S:178:ASP:O	1:S:204:HIS:HD2	1.71	0.73
1:C:147:LEU:HD13	1:C:235:ALA:HB2	1.70	0.73
1:B:243:SER:O	4:B:2154:HOH:O	2.06	0.73
1:S:28:ARG:HD2	4:S:2038:HOH:O	1.87	0.73
1:B:147:LEU:HD13	1:B:235:ALA:HB2	1.69	0.73
1:B:178:ASP:O	1:B:204:HIS:HD2	1.71	0.73
1:J:178:ASP:O	1:J:204:HIS:HD2	1.72	0.72
1:E:243:SER:O	4:E:2160:HOH:O	2.06	0.72
1:N:178:ASP:O	1:N:204:HIS:HD2	1.71	0.72
1:H:130:LYS:NZ	4:H:2101:HOH:O	2.10	0.72
1:I:178:ASP:O	1:I:204:HIS:HD2	1.71	0.72
1:N:147:LEU:HD13	1:N:235:ALA:HB2	1.70	0.72
1:R:28:ARG:HD2	4:R:2037:HOH:O	1.90	0.72
1:K:147:LEU:HD13	1:K:235:ALA:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:178:ASP:O	1:R:204:HIS:HD2	1.71	0.72
1:H:60:GLN:OE1	4:H:2068:HOH:O	0.72	0.71
1:K:248:LYS:NZ	4:K:2163:HOH:O	2.22	0.71
1:N:28:ARG:HD2	4:N:2036:HOH:O	1.90	0.71
1:T:147:LEU:HD13	1:T:235:ALA:HB2	1.71	0.71
1:J:46:HIS:HB2	4:J:2062:HOH:O	1.88	0.71
1:O:243:SER:O	4:O:2155:HOH:O	2.07	0.71
1:Q:147:LEU:HD13	1:Q:235:ALA:HB2	1.71	0.71
1:F:28:ARG:HD2	4:F:2037:HOH:O	1.91	0.71
1:M:178:ASP:O	1:M:204:HIS:HD2	1.74	0.71
1:E:147:LEU:HD13	1:E:235:ALA:HB2	1.71	0.70
1:F:248:LYS:NZ	4:F:2159:HOH:O	2.23	0.70
1:Q:248:LYS:NZ	4:Q:2166:HOH:O	2.23	0.70
1:Q:178:ASP:O	1:Q:204:HIS:HD2	1.73	0.70
1:F:147:LEU:HD13	1:F:235:ALA:HB2	1.73	0.70
1:S:243:SER:O	4:S:2151:HOH:O	2.09	0.70
1:H:178:ASP:O	1:H:204:HIS:HD2	1.75	0.70
1:K:28:ARG:HD2	4:K:2041:HOH:O	1.90	0.70
1:I:46:HIS:HE1	4:I:2063:HOH:O	1.75	0.70
1:R:147:LEU:HD13	1:R:235:ALA:HB2	1.72	0.70
1:L:248:LYS:NZ	4:L:2152:HOH:O	2.24	0.70
1:P:46:HIS:HE1	4:P:2050:HOH:O	1.73	0.70
1:J:243:SER:O	4:J:2158:HOH:O	2.09	0.69
1:B:46:HIS:HE1	4:B:2063:HOH:O	1.74	0.69
1:C:178:ASP:O	1:C:204:HIS:HD2	1.74	0.69
1:O:28:ARG:HD2	4:O:2037:HOH:O	1.91	0.69
1:R:243:SER:O	4:R:2152:HOH:O	2.09	0.69
1:B:28:ARG:HD2	4:B:2041:HOH:O	1.90	0.69
1:C:243:SER:O	4:C:2153:HOH:O	2.10	0.69
1:G:164:GLN:NE2	4:G:2116:HOH:O	2.24	0.69
1:J:147:LEU:HD13	1:J:235:ALA:HB2	1.73	0.69
1:T:46:HIS:HE1	4:T:2056:HOH:O	1.75	0.69
1:E:46:HIS:HE1	4:E:2066:HOH:O	1.76	0.68
1:D:164:GLN:NE2	4:D:2114:HOH:O	2.27	0.68
1:I:243:SER:O	4:I:2157:HOH:O	2.11	0.68
1:D:28:ARG:HD2	4:D:2039:HOH:O	1.93	0.68
1:N:67:ASN:HB2	4:N:2070:HOH:O	1.94	0.68
1:A:46:HIS:HE1	4:A:2065:HOH:O	1.77	0.67
1:G:28:ARG:HD2	4:G:2039:HOH:O	1.94	0.67
1:P:28:ARG:HD2	4:P:2034:HOH:O	1.93	0.67
1:O:164:GLN:NE2	4:O:2115:HOH:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:HIS:HE1	4:F:2058:HOH:O	1.78	0.67
1:K:247:MET:HE2	4:K:2119:HOH:O	1.92	0.67
1:G:243:SER:O	4:G:2156:HOH:O	2.13	0.67
1:A:243:SER:O	4:A:2158:HOH:O	2.13	0.67
1:M:243:SER:O	4:M:2163:HOH:O	2.12	0.67
1:O:67:ASN:HB2	4:O:2074:HOH:O	1.94	0.67
1:R:67:ASN:HB2	4:R:2074:HOH:O	1.95	0.67
1:S:202:GLN:HG2	4:S:2103:HOH:O	1.95	0.67
1:H:248:LYS:NZ	4:H:2157:HOH:O	2.27	0.67
1:D:67:ASN:HB2	4:D:2071:HOH:O	1.95	0.66
1:P:248:LYS:NZ	4:P:2152:HOH:O	2.27	0.66
1:T:164:GLN:NE2	4:T:2109:HOH:O	2.28	0.66
1:R:46:HIS:HE1	4:R:2061:HOH:O	1.77	0.66
1:S:46:HIS:HE1	4:S:2060:HOH:O	1.79	0.66
1:T:248:LYS:NZ	4:T:2155:HOH:O	2.22	0.66
1:J:46:HIS:HE1	4:J:2061:HOH:O	1.78	0.66
1:T:178:ASP:O	1:T:204:HIS:HD2	1.79	0.65
1:S:248:LYS:NZ	4:S:2156:HOH:O	2.30	0.65
1:Q:67:ASN:HB2	4:Q:2080:HOH:O	1.96	0.65
1:C:57:PRO:HD3	1:M:113:VAL:HG11	1.78	0.65
1:M:248:LYS:NZ	4:M:2170:HOH:O	2.29	0.65
1:S:127:GLU:OE1	4:S:2103:HOH:O	2.14	0.65
1:H:46:HIS:HE1	4:H:2056:HOH:O	1.78	0.64
1:M:46:HIS:HE1	4:M:2067:HOH:O	1.80	0.64
1:Q:164:GLN:NE2	1:Q:242:TYR:OH	2.31	0.64
1:G:46:HIS:HE1	4:G:2060:HOH:O	1.81	0.63
1:P:67:ASN:HB2	4:P:2064:HOH:O	1.97	0.63
1:I:67:ASN:HB2	4:I:2077:HOH:O	1.97	0.63
1:G:248:LYS:NZ	4:G:2162:HOH:O	2.20	0.63
1:L:46:HIS:HE1	4:L:2056:HOH:O	1.82	0.63
1:Q:64:LEU:HD23	1:Q:126:CYS:SG	2.38	0.63
1:E:28:ARG:HD2	4:E:2044:HOH:O	1.97	0.63
1:E:67:ASN:HB2	4:E:2080:HOH:O	1.99	0.63
1:K:46:HIS:HE1	4:K:2063:HOH:O	1.81	0.63
1:M:206:LEU:HD22	1:M:227:LEU:HD11	1.80	0.63
1:A:28:ARG:HD2	4:A:2044:HOH:O	1.99	0.62
1:C:28:ARG:HD2	4:D:2143:HOH:O	1.98	0.62
1:N:46:HIS:HE1	4:N:2057:HOH:O	1.81	0.62
1:K:137:ARG:HD3	4:K:2052:HOH:O	1.99	0.62
1:K:156:ASN:HB3	4:K:2114:HOH:O	1.99	0.62
1:T:28:ARG:HD2	4:T:2036:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LYS:NZ	4:C:2159:HOH:O	2.32	0.62
1:I:28:ARG:HD2	4:J:2148:HOH:O	1.99	0.62
1:J:67:ASN:HB2	4:J:2076:HOH:O	2.00	0.61
1:T:67:ASN:HB2	4:T:2070:HOH:O	1.99	0.61
1:I:248:LYS:NZ	4:I:2163:HOH:O	2.33	0.61
1:S:67:ASN:HB2	4:S:2074:HOH:O	1.99	0.61
1:L:67:ASN:HB2	4:L:2070:HOH:O	2.01	0.61
1:C:67:ASN:HB2	4:C:2076:HOH:O	2.00	0.61
1:H:164:GLN:NE2	4:H:2115:HOH:O	2.34	0.61
1:N:247:MET:HE2	4:N:2110:HOH:O	2.00	0.61
1:L:247:MET:HE2	4:L:2107:HOH:O	1.99	0.60
1:B:248:LYS:NZ	4:B:2160:HOH:O	2.23	0.60
1:Q:28:ARG:HD2	4:R:2143:HOH:O	2.01	0.60
1:F:67:ASN:HB2	4:F:2073:HOH:O	2.01	0.60
1:J:248:LYS:NZ	4:J:2163:HOH:O	2.32	0.60
1:M:164:GLN:NE2	4:M:2124:HOH:O	2.35	0.60
1:H:247:MET:HE2	4:H:2115:HOH:O	2.00	0.60
1:O:247:MET:HE2	4:O:2159:HOH:O	2.02	0.59
1:A:67:ASN:HB2	4:A:2079:HOH:O	2.01	0.59
1:C:13:MET:SD	1:C:33:LEU:HD13	2.43	0.59
1:T:247:MET:HE2	4:T:2154:HOH:O	2.02	0.59
1:G:67:ASN:HB2	4:G:2076:HOH:O	2.01	0.59
1:Q:247:MET:HE2	4:Q:2164:HOH:O	2.02	0.59
1:K:164:GLN:NE2	1:K:242:TYR:OH	2.35	0.59
1:N:156:ASN:HB3	4:N:2120:HOH:O	2.01	0.59
1:I:13:MET:SD	1:I:33:LEU:HD13	2.43	0.58
1:E:206:LEU:HD22	1:E:227:LEU:HD11	1.83	0.58
1:L:156:ASN:HB3	4:L:2116:HOH:O	2.03	0.58
1:F:156:ASN:HB3	4:F:2124:HOH:O	2.03	0.58
1:M:43:ALA:HB3	1:M:44:PRO:HD3	1.84	0.58
1:H:67:ASN:HB2	4:H:2072:HOH:O	2.03	0.58
1:L:164:GLN:NE2	4:L:2107:HOH:O	2.37	0.58
1:D:113:VAL:HG11	1:Q:57:PRO:HD3	1.86	0.57
1:L:180:VAL:HB	1:L:206:LEU:HB3	1.85	0.57
1:G:164:GLN:NE2	1:G:242:TYR:OH	2.36	0.57
1:Q:248:LYS:CE	4:Q:2166:HOH:O	2.52	0.57
1:E:248:LYS:NZ	4:E:2165:HOH:O	2.37	0.57
1:G:202:GLN:HG2	4:G:2104:HOH:O	2.04	0.57
1:C:46:HIS:HE1	4:C:2062:HOH:O	1.86	0.57
1:L:247:MET:HE2	4:L:2151:HOH:O	2.04	0.57
1:T:156:ASN:HB3	4:T:2118:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:206:LEU:HD22	1:Q:227:LEU:HD11	1.86	0.57
1:H:156:ASN:HB3	4:H:2108:HOH:O	2.05	0.56
1:P:180:VAL:HB	1:P:206:LEU:HB3	1.87	0.56
1:N:137:ARG:HD3	4:N:2049:HOH:O	2.05	0.56
1:R:13:MET:SD	1:R:33:LEU:HD13	2.45	0.56
1:T:157:ASP:CG	4:T:2104:HOH:O	2.38	0.56
1:E:164:GLN:NE2	4:E:2122:HOH:O	2.37	0.56
1:O:180:VAL:HB	1:O:206:LEU:HB3	1.87	0.56
1:S:137:ARG:HD3	4:S:2052:HOH:O	2.04	0.56
1:B:67:ASN:HB2	4:B:2076:HOH:O	2.05	0.56
1:K:164:GLN:NE2	4:K:2119:HOH:O	2.39	0.56
1:D:248:LYS:CE	4:D:2157:HOH:O	2.53	0.56
1:K:85:ASP:OD1	4:K:2085:HOH:O	2.18	0.56
1:P:247:MET:HE2	4:P:2151:HOH:O	2.05	0.56
1:O:164:GLN:NE2	1:O:242:TYR:OH	2.38	0.56
1:E:156:ASN:HB3	4:E:2130:HOH:O	2.05	0.56
1:L:13:MET:SD	1:L:33:LEU:HD13	2.45	0.55
1:P:247:MET:HE2	4:P:2106:HOH:O	2.06	0.55
1:N:248:LYS:CE	4:N:2155:HOH:O	2.54	0.55
1:G:156:ASN:HB3	4:G:2124:HOH:O	2.05	0.55
1:K:13:MET:SD	1:K:33:LEU:HD13	2.47	0.55
1:B:156:ASN:HB3	4:B:2123:HOH:O	2.07	0.55
1:M:137:ARG:HD3	4:M:2058:HOH:O	2.06	0.55
1:N:202:GLN:HG2	4:N:2099:HOH:O	2.06	0.55
1:K:206:LEU:HD22	1:K:227:LEU:HD11	1.89	0.55
1:O:206:LEU:HD22	1:O:227:LEU:HD11	1.88	0.55
1:M:67:ASN:HB2	4:M:2082:HOH:O	2.07	0.55
1:D:253:ARG:NH2	4:D:2161:HOH:O	2.38	0.55
1:O:46:HIS:CE1	4:O:2059:HOH:O	2.45	0.55
1:T:180:VAL:HB	1:T:206:LEU:HB3	1.89	0.55
1:F:206:LEU:HD22	1:F:227:LEU:HD11	1.89	0.55
1:H:13:MET:SD	1:H:33:LEU:HD13	2.47	0.54
1:K:1:MET:HB3	4:K:2065:HOH:O	2.07	0.54
1:D:103:HIS:ND1	4:D:2089:HOH:O	2.33	0.54
1:I:164:GLN:NE2	1:I:242:TYR:OH	2.40	0.54
1:O:13:MET:SD	1:O:33:LEU:HD13	2.47	0.54
1:Q:13:MET:SD	1:Q:33:LEU:HD13	2.47	0.54
1:A:64:LEU:HD23	1:A:126:CYS:SG	2.47	0.54
1:J:137:ARG:HD3	4:J:2052:HOH:O	2.07	0.54
1:L:206:LEU:HD22	1:L:227:LEU:HD11	1.89	0.54
1:F:247:MET:HE2	4:F:2115:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:247:MET:HE2	4:M:2124:HOH:O	2.08	0.54
1:P:137:ARG:HD3	4:P:2043:HOH:O	2.06	0.54
1:I:156:ASN:HB3	4:I:2126:HOH:O	2.07	0.53
1:N:206:LEU:HD22	1:N:227:LEU:HD11	1.90	0.53
1:J:206:LEU:HD22	1:J:227:LEU:HD11	1.90	0.53
1:E:13:MET:SD	1:E:33:LEU:HD13	2.48	0.53
1:G:180:VAL:HB	1:G:206:LEU:HB3	1.90	0.53
1:J:13:MET:SD	1:J:33:LEU:HD13	2.48	0.53
1:Q:203:LYS:NZ	4:Q:2135:HOH:O	2.32	0.53
1:F:13:MET:SD	1:F:33:LEU:HD13	2.49	0.53
1:O:248:LYS:CE	4:O:2160:HOH:O	2.54	0.53
1:S:164:GLN:NE2	1:S:242:TYR:OH	2.40	0.53
1:T:247:MET:HE2	4:T:2109:HOH:O	2.08	0.53
1:S:156:ASN:HB3	4:S:2123:HOH:O	2.09	0.53
1:B:13:MET:SD	1:B:33:LEU:HD13	2.49	0.53
1:O:247:MET:HE2	4:O:2115:HOH:O	2.06	0.53
1:E:43:ALA:HB3	1:E:44:PRO:HD3	1.91	0.52
1:E:137:ARG:HD3	4:E:2056:HOH:O	2.08	0.52
1:A:206:LEU:HD22	1:A:227:LEU:HD11	1.92	0.52
1:O:156:ASN:HB3	4:O:2124:HOH:O	2.08	0.52
1:C:137:ARG:HD3	4:C:2052:HOH:O	2.08	0.52
1:N:180:VAL:HB	1:N:206:LEU:HB3	1.90	0.52
1:R:180:VAL:HB	1:R:206:LEU:HB3	1.90	0.52
1:S:13:MET:SD	1:S:33:LEU:HD13	2.49	0.52
1:D:180:VAL:HB	1:D:206:LEU:HB3	1.91	0.52
1:L:164:GLN:NE2	1:L:242:TYR:OH	2.42	0.52
1:P:164:GLN:NE2	1:P:242:TYR:OH	2.42	0.52
1:S:206:LEU:HD22	1:S:227:LEU:HD11	1.91	0.52
1:D:13:MET:SD	1:D:33:LEU:HD13	2.49	0.52
1:G:247:MET:HE2	4:G:2116:HOH:O	2.09	0.52
1:N:164:GLN:NE2	1:N:242:TYR:OH	2.40	0.52
1:S:248:LYS:CE	4:S:2156:HOH:O	2.57	0.52
1:F:164:GLN:NE2	4:F:2115:HOH:O	2.43	0.52
1:A:137:ARG:HD3	4:A:2057:HOH:O	2.10	0.52
1:L:137:ARG:HD3	4:L:2047:HOH:O	2.08	0.52
1:R:247:MET:HE2	4:R:2110:HOH:O	2.08	0.52
1:A:13:MET:SD	1:A:33:LEU:HD13	2.49	0.52
1:H:163:ARG:NH2	1:H:274:LEU:C	2.68	0.52
1:I:43:ALA:HB3	1:I:44:PRO:HD3	1.92	0.52
1:C:156:ASN:HB3	4:C:2123:HOH:O	2.10	0.52
1:E:180:VAL:HB	1:E:206:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:13:MET:SD	1:N:33:LEU:HD13	2.49	0.52
1:T:64:LEU:HD23	1:T:126:CYS:SG	2.50	0.52
1:A:164:GLN:NE2	1:A:242:TYR:OH	2.40	0.51
1:E:247:MET:HE2	4:E:2122:HOH:O	2.10	0.51
1:F:54:ARG:HD3	4:F:2069:HOH:O	2.10	0.51
1:K:180:VAL:HB	1:K:206:LEU:HB3	1.91	0.51
1:S:164:GLN:NE2	4:S:2114:HOH:O	2.43	0.51
1:D:54:ARG:HD3	4:D:2066:HOH:O	2.08	0.51
1:K:248:LYS:CE	4:K:2163:HOH:O	2.56	0.51
1:C:180:VAL:HB	1:C:206:LEU:HB3	1.91	0.51
1:F:164:GLN:NE2	1:F:242:TYR:OH	2.41	0.51
1:L:202:GLN:HG2	4:L:2095:HOH:O	2.11	0.51
1:P:206:LEU:HD22	1:P:227:LEU:HD11	1.91	0.51
1:A:248:LYS:NZ	4:A:2163:HOH:O	2.35	0.51
1:G:247:MET:HE2	4:G:2160:HOH:O	2.11	0.51
1:P:54:ARG:HD3	4:P:2059:HOH:O	2.08	0.51
1:D:46:HIS:CE1	4:D:2055:HOH:O	2.50	0.51
1:B:164:GLN:NE2	1:B:242:TYR:OH	2.42	0.51
1:C:164:GLN:NE2	1:C:242:TYR:OH	2.40	0.51
1:C:164:GLN:NE2	4:C:2115:HOH:O	2.44	0.51
1:F:248:LYS:CE	4:F:2159:HOH:O	2.59	0.51
1:H:247:MET:HE2	4:H:2156:HOH:O	2.09	0.51
1:I:247:MET:HE2	4:I:2161:HOH:O	2.10	0.51
1:P:13:MET:SD	1:P:33:LEU:HD13	2.51	0.51
1:Q:46:HIS:CE1	4:Q:2065:HOH:O	2.49	0.51
1:T:164:GLN:NE2	1:T:242:TYR:OH	2.40	0.51
1:B:180:VAL:HB	1:B:206:LEU:HB3	1.92	0.51
1:M:13:MET:SD	1:M:33:LEU:HD13	2.51	0.51
1:D:247:MET:HE2	4:D:2156:HOH:O	2.12	0.50
1:O:155:GLU:HG3	4:P:2153:HOH:O	2.10	0.50
1:S:203:LYS:HB3	4:S:2127:HOH:O	2.11	0.50
1:B:248:LYS:CE	4:B:2160:HOH:O	2.58	0.50
1:H:137:ARG:HD3	4:H:2048:HOH:O	2.11	0.50
1:P:159:ALA:HB2	1:P:270:SER:HB2	1.93	0.50
1:B:43:ALA:HB3	1:B:44:PRO:HD3	1.93	0.50
1:D:164:GLN:NE2	1:D:242:TYR:OH	2.41	0.50
1:G:248:LYS:CE	4:G:2162:HOH:O	2.59	0.50
1:M:164:GLN:NE2	1:M:242:TYR:OH	2.38	0.50
1:R:164:GLN:NE2	4:R:2110:HOH:O	2.45	0.50
1:D:147:LEU:HD13	1:D:235:ALA:CB	2.37	0.50
1:H:58:LEU:HG	1:H:62:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:VAL:HB	1:J:206:LEU:HB3	1.94	0.50
1:Q:180:VAL:HB	1:Q:206:LEU:HB3	1.94	0.50
1:H:248:LYS:CE	4:H:2157:HOH:O	2.60	0.50
1:I:180:VAL:HB	1:I:206:LEU:HB3	1.93	0.49
1:J:164:GLN:NE2	1:J:242:TYR:OH	2.43	0.49
1:L:43:ALA:HB3	1:L:44:PRO:HD3	1.92	0.49
1:T:206:LEU:HD22	1:T:227:LEU:HD11	1.94	0.49
1:B:164:GLN:NE2	4:B:2115:HOH:O	2.45	0.49
1:E:64:LEU:HD23	1:E:126:CYS:SG	2.52	0.49
1:E:248:LYS:CE	4:E:2165:HOH:O	2.59	0.49
1:H:206:LEU:HD22	1:H:227:LEU:HD11	1.93	0.49
1:A:1:MET:HB3	4:A:2069:HOH:O	2.12	0.49
1:M:180:VAL:HB	1:M:206:LEU:HB3	1.94	0.49
1:R:156:ASN:HB3	4:R:2119:HOH:O	2.12	0.49
1:P:1:MET:HB3	4:P:2053:HOH:O	2.12	0.49
1:P:156:ASN:HB3	4:P:2114:HOH:O	2.12	0.49
1:I:164:GLN:NE2	4:I:2118:HOH:O	2.44	0.49
1:L:248:LYS:CE	4:L:2152:HOH:O	2.61	0.49
1:R:248:LYS:NZ	4:R:2157:HOH:O	2.13	0.49
1:A:247:MET:HE2	4:A:2161:HOH:O	2.12	0.49
1:A:180:VAL:HB	1:A:206:LEU:HB3	1.95	0.49
1:F:180:VAL:HB	1:F:206:LEU:HB3	1.94	0.49
1:P:43:ALA:HB3	1:P:44:PRO:HD3	1.95	0.49
1:P:248:LYS:CE	4:P:2152:HOH:O	2.59	0.49
1:G:13:MET:SD	1:G:33:LEU:HD13	2.53	0.48
1:L:147:LEU:HD13	1:L:235:ALA:CB	2.41	0.48
1:T:13:MET:SD	1:T:33:LEU:HD13	2.53	0.48
1:A:127:GLU:OE1	4:A:2106:HOH:O	2.20	0.48
1:F:202:GLN:HG2	4:F:2103:HOH:O	2.12	0.48
1:K:58:LEU:HG	1:K:62:MET:HE3	1.96	0.48
1:O:173:LEU:HD21	1:O:267:PRO:HB3	1.96	0.48
1:T:248:LYS:CE	4:T:2155:HOH:O	2.59	0.48
1:H:180:VAL:HB	1:H:206:LEU:HB3	1.94	0.48
1:K:202:GLN:HG2	4:K:2107:HOH:O	2.13	0.48
1:J:247:MET:HE2	4:J:2117:HOH:O	2.14	0.48
1:K:43:ALA:HB3	1:K:44:PRO:HD3	1.95	0.48
1:M:54:ARG:HD3	4:M:2076:HOH:O	2.12	0.48
1:Q:2:GLN:HG3	4:Q:2003:HOH:O	2.13	0.48
1:T:43:ALA:HB3	1:T:44:PRO:HD3	1.95	0.48
1:G:147:LEU:HD13	1:G:235:ALA:CB	2.42	0.48
1:R:248:LYS:CE	4:R:2157:HOH:O	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LEU:HD22	1:C:227:LEU:HD11	1.95	0.48
1:E:1:MET:HB3	4:E:2069:HOH:O	2.13	0.48
1:N:54:ARG:HD3	4:N:2065:HOH:O	2.12	0.48
1:I:54:ARG:HD3	4:I:2072:HOH:O	2.14	0.48
1:T:202:GLN:HG2	4:T:2094:HOH:O	2.12	0.48
1:A:57:PRO:HD3	1:E:113:VAL:HG11	1.96	0.48
1:B:1:MET:HB3	4:B:2065:HOH:O	2.13	0.48
1:B:203:LYS:NZ	4:B:2129:HOH:O	2.42	0.48
1:C:113:VAL:HG11	1:M:57:PRO:HD3	1.94	0.48
1:M:156:ASN:HB3	4:M:2118:HOH:O	2.13	0.48
1:Q:156:ASN:HB3	4:Q:2129:HOH:O	2.13	0.48
1:D:156:ASN:HB3	4:D:2120:HOH:O	2.14	0.47
1:K:203:LYS:HE3	1:K:203:LYS:HB2	1.62	0.47
1:Q:43:ALA:HB3	1:Q:44:PRO:HD3	1.95	0.47
1:Q:247:MET:HE2	4:Q:2120:HOH:O	2.13	0.47
1:F:137:ARG:HD3	4:F:2050:HOH:O	2.14	0.47
1:I:202:GLN:HG2	4:I:2107:HOH:O	2.14	0.47
1:R:206:LEU:HD22	1:R:227:LEU:HD11	1.94	0.47
1:T:2:GLN:HG3	4:T:2002:HOH:O	2.14	0.47
1:L:203:LYS:HB2	1:L:203:LYS:HE3	1.66	0.47
1:M:1:MET:HB3	4:M:2070:HOH:O	2.14	0.47
1:T:46:HIS:CE1	4:T:2056:HOH:O	2.57	0.47
1:S:180:VAL:HB	1:S:206:LEU:HB3	1.95	0.47
1:L:212:HIS:CD2	1:L:212:HIS:C	2.92	0.47
1:T:137:ARG:HD3	4:T:2047:HOH:O	2.13	0.47
1:J:203:LYS:HB2	1:J:203:LYS:HE3	1.71	0.47
1:A:156:ASN:HB3	4:A:2127:HOH:O	2.15	0.47
1:E:164:GLN:NE2	1:E:242:TYR:OH	2.42	0.47
1:J:1:MET:HB3	4:J:2065:HOH:O	2.15	0.47
1:J:212:HIS:C	1:J:212:HIS:CD2	2.90	0.47
1:N:43:ALA:HB3	1:N:44:PRO:HD3	1.97	0.47
1:P:46:HIS:CE1	4:P:2050:HOH:O	2.57	0.47
1:P:202:GLN:HG2	4:P:2095:HOH:O	2.14	0.47
1:C:64:LEU:HD23	1:C:126:CYS:SG	2.55	0.47
1:P:212:HIS:C	1:P:212:HIS:CD2	2.90	0.47
1:A:202:GLN:HG2	4:A:2106:HOH:O	2.15	0.47
1:C:1:MET:HB3	4:C:2063:HOH:O	2.15	0.47
1:G:136:ASP:OD1	4:G:2106:HOH:O	2.20	0.47
1:J:202:GLN:HG2	4:J:2104:HOH:O	2.14	0.47
1:S:195:GLN:O	1:S:199:GLN:HB2	2.15	0.47
1:A:203:LYS:HE3	1:A:203:LYS:HB2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:LEU:HD22	1:I:227:LEU:HD11	1.96	0.47
1:R:164:GLN:NE2	1:R:242:TYR:OH	2.42	0.47
1:B:57:PRO:HD3	1:I:113:VAL:HG11	1.97	0.46
1:B:64:LEU:HD23	1:B:126:CYS:SG	2.56	0.46
1:H:164:GLN:NE2	1:H:242:TYR:OH	2.41	0.46
1:J:159:ALA:HB2	1:J:270:SER:HB2	1.98	0.46
1:G:206:LEU:HD22	1:G:227:LEU:HD11	1.97	0.46
1:I:2:GLN:HG3	4:I:2003:HOH:O	2.15	0.46
1:A:128:ARG:HG3	1:A:217:SER:OG	2.15	0.46
1:C:54:ARG:HD3	4:C:2071:HOH:O	2.13	0.46
1:J:80:ARG:O	1:J:80:ARG:HD3	2.15	0.46
1:K:212:HIS:C	1:K:212:HIS:CD2	2.92	0.46
1:O:27:GLU:O	1:O:28:ARG:C	2.57	0.46
1:S:52:GLN:CD	1:S:52:GLN:H	2.23	0.46
1:B:118:LEU:N	1:B:119:PRO:CD	2.78	0.46
1:G:159:ALA:HB2	1:G:270:SER:HB2	1.97	0.46
1:H:1:MET:HB3	4:H:2058:HOH:O	2.15	0.46
1:L:83:GLN:HG3	1:L:84:LEU:HD13	1.98	0.46
1:R:159:ALA:HB2	1:R:270:SER:HB2	1.98	0.46
1:H:203:LYS:HB2	1:H:203:LYS:HE3	1.62	0.46
1:K:159:ALA:HB2	1:K:270:SER:HB2	1.98	0.46
1:O:212:HIS:C	1:O:212:HIS:CD2	2.93	0.46
1:T:159:ALA:HB2	1:T:270:SER:HB2	1.96	0.46
1:C:202:GLN:HG2	4:C:2103:HOH:O	2.16	0.46
1:H:2:GLN:HG3	4:H:2002:HOH:O	2.16	0.46
1:N:46:HIS:CE1	4:N:2057:HOH:O	2.63	0.46
1:R:248:LYS:HD2	4:R:2157:HOH:O	2.16	0.46
1:G:137:ARG:HD3	4:G:2053:HOH:O	2.14	0.46
1:N:164:GLN:NE2	4:N:2110:HOH:O	2.49	0.46
1:C:118:LEU:N	1:C:119:PRO:CD	2.79	0.46
1:G:43:ALA:HB3	1:G:44:PRO:HD3	1.98	0.46
1:P:2:GLN:HG3	4:P:2002:HOH:O	2.15	0.46
1:E:247:MET:HE2	4:E:2164:HOH:O	2.16	0.46
1:F:64:LEU:HD23	1:F:126:CYS:SG	2.56	0.46
1:J:54:ARG:HD3	4:J:2070:HOH:O	2.16	0.46
1:K:83:GLN:HG3	1:K:84:LEU:HD13	1.98	0.46
1:N:212:HIS:C	1:N:212:HIS:CD2	2.94	0.46
1:O:52:GLN:O	1:O:53:PRO:C	2.59	0.46
1:T:124:SER:HB3	1:T:201:MET:HG3	1.98	0.46
1:G:124:SER:HB3	1:G:201:MET:HG3	1.98	0.45
1:I:203:LYS:HB2	1:I:203:LYS:HE3	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:173:LEU:HD21	1:N:267:PRO:HB3	1.98	0.45
1:O:124:SER:HB3	1:O:201:MET:HG3	1.97	0.45
1:O:203:LYS:HB2	1:O:203:LYS:HE3	1.66	0.45
4:Q:2165:HOH:O	1:T:155:GLU:HG3	2.16	0.45
1:A:118:LEU:N	1:A:119:PRO:CD	2.80	0.45
1:I:64:LEU:HD23	1:I:126:CYS:SG	2.56	0.45
1:M:58:LEU:HD12	1:M:58:LEU:HA	1.79	0.45
1:M:202:GLN:HG2	4:M:2111:HOH:O	2.16	0.45
1:S:124:SER:HB3	1:S:201:MET:HG3	1.98	0.45
1:M:163:ARG:NH2	1:M:274:LEU:C	2.74	0.45
1:B:248:LYS:HD2	4:B:2160:HOH:O	2.15	0.45
1:H:118:LEU:N	1:H:119:PRO:CD	2.80	0.45
1:I:247:MET:HE2	4:I:2118:HOH:O	2.16	0.45
1:D:57:PRO:HD3	1:Q:113:VAL:HG11	1.97	0.45
1:D:206:LEU:HD22	1:D:227:LEU:HD11	1.98	0.45
1:E:1:MET:HA	4:E:2002:HOH:O	2.16	0.45
1:I:261:LYS:HE2	1:I:261:LYS:HB3	1.80	0.45
1:J:164:GLN:NE2	4:J:2117:HOH:O	2.49	0.45
1:B:206:LEU:HD22	1:B:227:LEU:HD11	1.99	0.45
1:C:247:MET:HE2	4:C:2115:HOH:O	2.16	0.45
1:M:173:LEU:HD21	1:M:267:PRO:HB3	1.98	0.45
1:S:52:GLN:O	1:S:53:PRO:C	2.60	0.45
1:S:212:HIS:C	1:S:212:HIS:CD2	2.94	0.45
1:H:43:ALA:HB3	1:H:44:PRO:HD3	1.97	0.45
1:I:159:ALA:HB2	1:I:270:SER:HB2	1.98	0.45
1:O:2:GLN:HG3	4:O:2002:HOH:O	2.16	0.45
1:A:43:ALA:HB3	1:A:44:PRO:HD3	1.97	0.45
1:C:212:HIS:C	1:C:212:HIS:CD2	2.95	0.45
1:H:212:HIS:C	1:H:212:HIS:CD2	2.95	0.45
1:J:173:LEU:HD21	1:J:267:PRO:HB3	1.98	0.45
1:B:203:LYS:HB2	1:B:203:LYS:HE3	1.66	0.45
1:P:203:LYS:HE3	1:P:203:LYS:HB2	1.65	0.45
1:Q:261:LYS:HE2	1:Q:261:LYS:HB3	1.86	0.45
1:E:157:ASP:O	1:E:158:THR:C	2.57	0.45
1:G:27:GLU:O	1:G:28:ARG:C	2.60	0.45
1:G:64:LEU:HD23	1:G:126:CYS:SG	2.56	0.45
1:S:247:MET:HE2	4:S:2114:HOH:O	2.16	0.45
1:D:247:MET:HE2	4:D:2114:HOH:O	2.17	0.44
1:K:173:LEU:HD21	1:K:267:PRO:HB3	1.99	0.44
1:M:2:GLN:HG3	4:M:2003:HOH:O	2.17	0.44
1:H:124:SER:HB3	1:H:201:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:52:GLN:O	1:I:53:PRO:C	2.60	0.44
1:M:212:HIS:C	1:M:212:HIS:CD2	2.95	0.44
1:B:212:HIS:C	1:B:212:HIS:CD2	2.95	0.44
1:B:247:MET:HE2	4:B:2158:HOH:O	2.16	0.44
1:C:43:ALA:HB3	1:C:44:PRO:HD3	2.00	0.44
1:E:261:LYS:HE2	1:E:261:LYS:HB3	1.91	0.44
4:E:2166:HOH:O	1:H:155:GLU:HG3	2.16	0.44
1:A:164:GLN:NE2	4:A:2118:HOH:O	2.49	0.44
1:G:178:ASP:O	1:G:204:HIS:CD2	2.55	0.44
1:H:247:MET:HE3	1:H:247:MET:HB2	1.89	0.44
1:I:248:LYS:CE	4:I:2163:HOH:O	2.64	0.44
1:J:28:ARG:HG3	1:K:226:GLY:HA3	1.99	0.44
1:J:43:ALA:HB3	1:J:44:PRO:HD3	1.98	0.44
1:J:156:ASN:HB3	4:J:2125:HOH:O	2.16	0.44
1:K:54:ARG:HD3	4:K:2073:HOH:O	2.17	0.44
1:M:203:LYS:HE3	1:M:203:LYS:HB2	1.64	0.44
1:N:178:ASP:O	1:N:204:HIS:CD2	2.62	0.44
1:O:64:LEU:HD23	1:O:126:CYS:SG	2.58	0.44
1:P:214:VAL:HG22	1:P:215:PHE:N	2.32	0.44
1:A:248:LYS:CE	4:A:2163:HOH:O	2.64	0.44
1:D:202:GLN:HG2	4:D:2099:HOH:O	2.18	0.44
1:E:177:PRO:HB3	1:E:265:VAL:HG13	1.99	0.44
1:B:27:GLU:O	1:B:28:ARG:C	2.59	0.44
1:J:64:LEU:HD23	1:J:126:CYS:SG	2.57	0.44
1:N:159:ALA:HB2	1:N:270:SER:HB2	1.98	0.44
1:C:248:LYS:CE	4:C:2159:HOH:O	2.66	0.44
1:K:261:LYS:HE2	1:K:261:LYS:HB3	1.84	0.44
1:S:43:ALA:HB3	1:S:44:PRO:HD3	1.99	0.44
1:A:113:VAL:HG11	1:E:57:PRO:HD3	2.00	0.44
1:B:137:ARG:HD3	4:B:2053:HOH:O	2.18	0.44
1:I:124:SER:HB3	1:I:201:MET:HG3	1.99	0.44
1:M:248:LYS:HD2	4:M:2170:HOH:O	2.17	0.44
1:O:157:ASP:O	1:O:158:THR:C	2.61	0.44
1:P:178:ASP:O	1:P:204:HIS:CD2	2.60	0.44
1:T:212:HIS:C	1:T:212:HIS:CD2	2.95	0.44
1:H:28:ARG:HB3	1:H:29:ASN:H	1.58	0.44
1:H:83:GLN:HG3	1:H:84:LEU:HD13	1.99	0.44
1:I:1:MET:HA	4:I:2002:HOH:O	2.18	0.44
1:P:173:LEU:HD21	1:P:267:PRO:HB3	2.00	0.44
1:P:248:LYS:HD2	4:P:2152:HOH:O	2.18	0.44
1:A:262:ARG:HG3	1:A:262:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:THR:OG1	3:H:300:PGH:O2P	2.25	0.43
1:S:28:ARG:HG3	1:T:226:GLY:HA3	1.99	0.43
1:B:54:ARG:HD3	4:B:2071:HOH:O	2.17	0.43
1:B:159:ALA:HB2	1:B:270:SER:HB2	2.01	0.43
1:J:52:GLN:CD	1:J:52:GLN:H	2.26	0.43
1:L:64:LEU:HD23	1:L:126:CYS:SG	2.58	0.43
1:L:247:MET:HE3	1:L:247:MET:HB2	1.87	0.43
1:O:247:MET:HE3	1:O:247:MET:HB2	1.85	0.43
1:R:202:GLN:HG2	4:R:2099:HOH:O	2.18	0.43
1:A:248:LYS:HD2	4:A:2163:HOH:O	2.17	0.43
1:D:212:HIS:CD2	1:D:212:HIS:C	2.96	0.43
1:F:212:HIS:C	1:F:212:HIS:CD2	2.96	0.43
1:P:164:GLN:NE2	4:P:2106:HOH:O	2.49	0.43
1:C:27:GLU:O	1:C:28:ARG:C	2.61	0.43
1:C:52:GLN:CD	1:C:52:GLN:H	2.26	0.43
1:D:124:SER:HB3	1:D:201:MET:HG3	2.00	0.43
1:E:173:LEU:HD21	1:E:267:PRO:HB3	2.00	0.43
1:H:46:HIS:CE1	4:H:2056:HOH:O	2.63	0.43
1:J:28:ARG:HB3	1:J:29:ASN:H	1.61	0.43
1:K:157:ASP:O	1:K:158:THR:C	2.61	0.43
1:L:27:GLU:O	1:L:27:GLU:HG2	2.17	0.43
1:A:157:ASP:O	1:A:158:THR:C	2.61	0.43
1:A:212:HIS:C	1:A:212:HIS:CD2	2.95	0.43
1:I:58:LEU:HD12	1:I:58:LEU:HA	1.85	0.43
1:J:52:GLN:O	1:J:53:PRO:C	2.61	0.43
1:J:214:VAL:HG22	1:J:215:PHE:N	2.33	0.43
1:M:248:LYS:CE	4:M:2170:HOH:O	2.65	0.43
1:M:261:LYS:HE2	1:M:261:LYS:HB3	1.92	0.43
1:R:49:PHE:N	1:R:49:PHE:CD1	2.86	0.43
1:S:27:GLU:O	1:S:28:ARG:C	2.60	0.43
1:S:159:ALA:HB2	1:S:270:SER:HB2	2.00	0.43
1:T:54:ARG:HD3	4:T:2065:HOH:O	2.19	0.43
1:D:60:GLN:HB2	1:R:262:ARG:HD2	1.99	0.43
1:D:178:ASP:O	1:D:204:HIS:CD2	2.61	0.43
1:D:203:LYS:NZ	4:D:2126:HOH:O	2.50	0.43
1:G:203:LYS:HB2	1:G:203:LYS:HE3	1.75	0.43
1:G:212:HIS:C	1:G:212:HIS:CD2	2.96	0.43
1:L:163:ARG:NH2	1:L:274:LEU:C	2.76	0.43
1:N:58:LEU:HD12	1:N:58:LEU:HA	1.83	0.43
1:B:202:GLN:HG2	4:B:2103:HOH:O	2.18	0.43
1:J:58:LEU:HG	1:J:62:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:147:LEU:HG	1:O:208:LEU:HD21	2.01	0.43
1:P:58:LEU:HG	1:P:62:MET:HE3	1.99	0.43
1:I:173:LEU:HD21	1:I:267:PRO:HB3	2.00	0.43
1:M:1:MET:HA	4:M:2002:HOH:O	2.19	0.43
1:O:49:PHE:N	1:O:49:PHE:CD1	2.87	0.43
1:P:124:SER:HB3	1:P:201:MET:HG3	2.00	0.43
1:A:28:ARG:HB3	1:A:29:ASN:H	1.58	0.42
1:E:212:HIS:C	1:E:212:HIS:CD2	2.96	0.42
1:F:147:LEU:HG	1:F:208:LEU:HD21	2.01	0.42
1:H:147:LEU:HD13	1:H:235:ALA:CB	2.47	0.42
1:J:247:MET:HE2	4:J:2162:HOH:O	2.19	0.42
1:S:163:ARG:HD2	1:S:167:GLU:OE2	2.19	0.42
1:E:203:LYS:HB2	1:E:203:LYS:HE3	1.74	0.42
1:F:83:GLN:HG3	1:F:84:LEU:HD13	2.00	0.42
1:G:52:GLN:O	1:G:53:PRO:C	2.63	0.42
1:N:247:MET:HE3	1:N:247:MET:HB2	1.92	0.42
1:Q:212:HIS:C	1:Q:212:HIS:CD2	2.97	0.42
1:A:46:HIS:CE1	4:A:2065:HOH:O	2.62	0.42
1:D:137:ARG:HD3	4:D:2047:HOH:O	2.18	0.42
1:F:46:HIS:CE1	4:F:2058:HOH:O	2.62	0.42
1:F:173:LEU:HD21	1:F:267:PRO:HB3	2.01	0.42
1:I:226:GLY:HA3	1:L:28:ARG:HG3	2.01	0.42
1:K:1:MET:N	4:K:2001:HOH:O	2.53	0.42
1:N:247:MET:HE2	4:N:2154:HOH:O	2.18	0.42
1:R:52:GLN:O	1:R:53:PRO:C	2.62	0.42
1:R:212:HIS:C	1:R:212:HIS:CD2	2.96	0.42
1:A:147:LEU:HG	1:A:208:LEU:HD21	2.01	0.42
1:M:247:MET:HE2	4:M:2167:HOH:O	2.19	0.42
1:N:147:LEU:HG	1:N:208:LEU:HD21	2.01	0.42
1:N:203:LYS:HB2	1:N:203:LYS:HE3	1.80	0.42
1:Q:54:ARG:HD3	4:Q:2075:HOH:O	2.19	0.42
1:R:261:LYS:HE2	1:R:261:LYS:HB3	1.90	0.42
1:A:147:LEU:HD13	1:A:235:ALA:CB	2.44	0.42
1:D:247:MET:HE3	1:D:247:MET:HB2	1.95	0.42
1:G:163:ARG:HD2	1:G:167:GLU:OE2	2.18	0.42
1:I:118:LEU:N	1:I:119:PRO:CD	2.82	0.42
1:J:261:LYS:HE2	1:J:261:LYS:HB3	1.91	0.42
1:L:178:ASP:O	1:L:204:HIS:CD2	2.61	0.42
1:R:173:LEU:HD21	1:R:267:PRO:HB3	2.01	0.42
1:C:203:LYS:HE2	4:C:2127:HOH:O	2.20	0.42
1:F:43:ALA:N	1:F:44:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:LEU:HD12	1:G:58:LEU:HA	1.83	0.42
1:L:52:GLN:O	1:L:53:PRO:C	2.62	0.42
1:M:114:PRO:O	1:M:115:THR:C	2.63	0.42
1:M:118:LEU:N	1:M:119:PRO:CD	2.83	0.42
1:S:118:LEU:N	1:S:119:PRO:CD	2.82	0.42
1:H:52:GLN:CD	1:H:52:GLN:H	2.27	0.42
1:I:137:ARG:HD3	4:I:2053:HOH:O	2.20	0.42
1:K:27:GLU:O	1:K:28:ARG:C	2.63	0.42
1:M:27:GLU:O	1:M:27:GLU:HG2	2.20	0.42
1:N:195:GLN:O	1:N:199:GLN:HB2	2.20	0.42
1:T:203:LYS:HB2	1:T:203:LYS:HE3	1.64	0.42
1:I:28:ARG:HB3	1:I:29:ASN:H	1.53	0.42
1:L:49:PHE:N	1:L:49:PHE:CD1	2.87	0.42
1:O:83:GLN:HG3	1:O:84:LEU:HD13	2.02	0.42
1:Q:52:GLN:H	1:Q:52:GLN:CD	2.28	0.42
1:Q:177:PRO:HB3	1:Q:265:VAL:HG13	2.01	0.42
1:R:52:GLN:CD	1:R:52:GLN:H	2.28	0.42
1:T:28:ARG:HB3	1:T:29:ASN:H	1.66	0.42
1:F:159:ALA:HB2	1:F:270:SER:HB2	2.02	0.42
1:H:9:PHE:HE1	1:H:92:ILE:HD11	1.85	0.42
1:K:114:PRO:O	1:K:115:THR:C	2.63	0.42
1:L:157:ASP:O	1:L:158:THR:C	2.63	0.42
1:N:203:LYS:HE2	4:N:2124:HOH:O	2.19	0.42
1:R:43:ALA:N	1:R:44:PRO:CD	2.82	0.42
1:R:60:GLN:HA	1:R:61:PRO:HD3	1.96	0.42
1:A:159:ALA:HB2	1:A:270:SER:HB2	2.02	0.41
1:G:83:GLN:HG3	1:G:84:LEU:HD13	2.02	0.41
1:G:261:LYS:HE2	1:G:261:LYS:HB3	1.89	0.41
1:K:177:PRO:HB3	1:K:265:VAL:HG13	2.01	0.41
1:K:247:MET:HE2	4:K:2161:HOH:O	2.19	0.41
1:P:28:ARG:HB3	1:P:29:ASN:H	1.64	0.41
1:C:28:ARG:HB3	1:C:29:ASN:H	1.55	0.41
1:F:28:ARG:HB3	1:F:29:ASN:H	1.60	0.41
1:J:27:GLU:O	1:J:28:ARG:C	2.61	0.41
1:N:83:GLN:HG3	1:N:84:LEU:HD13	2.01	0.41
1:O:137:ARG:HD3	4:O:2051:HOH:O	2.19	0.41
1:O:159:ALA:HB2	1:O:270:SER:HB2	2.01	0.41
1:Q:43:ALA:N	1:Q:44:PRO:CD	2.82	0.41
1:D:83:GLN:HG3	1:D:84:LEU:HD13	2.02	0.41
1:E:202:GLN:HG2	4:E:2110:HOH:O	2.19	0.41
1:G:157:ASP:O	1:G:158:THR:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:LEU:N	1:K:119:PRO:CD	2.84	0.41
1:N:64:LEU:HD23	1:N:126:CYS:SG	2.60	0.41
1:O:28:ARG:HB3	1:O:29:ASN:H	1.55	0.41
1:O:118:LEU:N	1:O:119:PRO:CD	2.84	0.41
1:A:52:GLN:O	1:A:53:PRO:C	2.62	0.41
1:D:203:LYS:HE3	1:D:203:LYS:HB2	1.72	0.41
1:G:52:GLN:H	1:G:52:GLN:CD	2.28	0.41
1:K:147:LEU:HG	1:K:208:LEU:HD21	2.02	0.41
1:M:274:LEU:HD12	1:M:274:LEU:HA	1.87	0.41
1:C:247:MET:HE3	1:C:247:MET:HB2	1.95	0.41
1:D:214:VAL:HG22	1:D:215:PHE:N	2.36	0.41
1:D:248:LYS:HD2	4:D:2157:HOH:O	2.21	0.41
1:M:64:LEU:HD23	1:M:126:CYS:SG	2.59	0.41
1:A:124:SER:HB3	1:A:201:MET:HG3	2.03	0.41
1:C:60:GLN:HA	1:C:61:PRO:HD3	1.94	0.41
1:F:52:GLN:O	1:F:53:PRO:C	2.62	0.41
1:J:60:GLN:HA	1:J:61:PRO:HD3	1.96	0.41
1:N:27:GLU:O	1:N:28:ARG:C	2.64	0.41
1:N:49:PHE:N	1:N:49:PHE:CD1	2.88	0.41
1:R:203:LYS:HE3	1:R:203:LYS:HB2	1.67	0.41
1:S:247:MET:HE2	4:S:2155:HOH:O	2.20	0.41
1:A:261:LYS:HE2	1:A:261:LYS:HB3	1.87	0.41
1:B:177:PRO:HB3	1:B:265:VAL:HG13	2.02	0.41
1:C:177:PRO:HB3	1:C:265:VAL:HG13	2.02	0.41
1:I:1:MET:HB3	4:I:2066:HOH:O	2.20	0.41
1:M:177:PRO:HB3	1:M:265:VAL:HG13	2.02	0.41
1:N:60:GLN:HA	1:N:61:PRO:HD3	1.97	0.41
1:N:177:PRO:HB3	1:N:265:VAL:HG13	2.02	0.41
1:O:1:MET:HG3	1:O:2:GLN:O	2.21	0.41
1:O:43:ALA:HB3	1:O:44:PRO:HD3	2.01	0.41
1:P:118:LEU:N	1:P:119:PRO:CD	2.82	0.41
1:Q:247:MET:HE3	1:Q:247:MET:HB2	1.93	0.41
1:R:214:VAL:HG22	1:R:215:PHE:N	2.36	0.41
1:T:163:ARG:HD2	1:T:167:GLU:OE2	2.20	0.41
1:B:52:GLN:O	1:B:53:PRO:C	2.62	0.41
1:C:214:VAL:HG22	1:C:215:PHE:N	2.36	0.41
1:G:173:LEU:HD21	1:G:267:PRO:HB3	2.02	0.41
1:J:163:ARG:HD2	1:J:167:GLU:OE2	2.20	0.41
1:P:52:GLN:O	1:P:53:PRO:C	2.62	0.41
1:Q:157:ASP:O	1:Q:158:THR:C	2.63	0.41
1:Q:214:VAL:HG22	1:Q:215:PHE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:HB2	1:D:270:SER:HB2	2.03	0.41
1:E:118:LEU:N	1:E:119:PRO:CD	2.84	0.41
1:H:159:ALA:HB2	1:H:270:SER:HB2	2.02	0.41
1:I:78:PHE:O	1:I:79:PHE:C	2.64	0.41
1:I:212:HIS:C	1:I:212:HIS:CD2	2.99	0.41
1:M:27:GLU:O	1:M:28:ARG:C	2.64	0.41
1:M:52:GLN:O	1:M:53:PRO:C	2.63	0.41
1:M:52:GLN:CD	1:M:52:GLN:H	2.28	0.41
1:M:247:MET:HE3	1:M:247:MET:HB2	1.97	0.41
1:N:28:ARG:HB3	1:N:29:ASN:H	1.58	0.41
1:P:64:LEU:HD23	1:P:126:CYS:SG	2.61	0.41
1:Q:137:ARG:HD3	4:Q:2056:HOH:O	2.20	0.41
1:R:137:ARG:HD3	4:R:2052:HOH:O	2.20	0.41
1:T:157:ASP:O	1:T:158:THR:C	2.60	0.41
1:B:61:PRO:HD2	1:J:262:ARG:O	2.21	0.41
1:D:2:GLN:HG3	4:D:2003:HOH:O	2.20	0.41
1:H:54:ARG:HD3	4:H:2066:HOH:O	2.21	0.40
1:L:128:ARG:HA	1:L:128:ARG:HD2	1.90	0.40
1:L:159:ALA:HB2	1:L:270:SER:HB2	2.03	0.40
1:P:60:GLN:HA	1:P:61:PRO:HD3	1.96	0.40
1:T:58:LEU:HG	1:T:62:MET:HE3	2.03	0.40
1:A:169:SER:O	1:A:170:THR:C	2.64	0.40
1:B:28:ARG:HB3	1:B:29:ASN:H	1.65	0.40
1:E:135:LYS:NZ	1:E:135:LYS:HB3	2.36	0.40
1:E:247:MET:HE3	1:E:247:MET:HB2	1.96	0.40
1:G:28:ARG:HB3	1:G:29:ASN:H	1.59	0.40
1:T:52:GLN:O	1:T:53:PRO:C	2.62	0.40
1:A:177:PRO:HB3	1:A:265:VAL:HG13	2.03	0.40
1:C:173:LEU:HD21	1:C:267:PRO:HB3	2.03	0.40
1:J:147:LEU:HG	1:J:208:LEU:HD21	2.03	0.40
1:N:261:LYS:HE2	1:N:261:LYS:HB3	1.91	0.40
1:O:54:ARG:HD3	4:O:2068:HOH:O	2.20	0.40
1:O:214:VAL:HG22	1:O:215:PHE:N	2.36	0.40
1:I:163:ARG:HD2	1:I:167:GLU:OE2	2.21	0.40
1:J:118:LEU:N	1:J:119:PRO:CD	2.84	0.40
1:K:2:GLN:HG3	4:K:2003:HOH:O	2.21	0.40
1:T:195:GLN:O	1:T:199:GLN:HB2	2.21	0.40
1:T:248:LYS:HD2	4:T:2155:HOH:O	2.21	0.40
1:A:2:GLN:HG3	4:A:2004:HOH:O	2.21	0.40
1:J:248:LYS:CE	4:J:2163:HOH:O	2.69	0.40
1:M:60:GLN:HA	1:M:61:PRO:HD3	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:262:ARG:HH11	1:R:262:ARG:HG3	1.86	0.40
1:S:1:MET:HB3	4:S:2063:HOH:O	2.22	0.40
1:S:54:ARG:HD3	4:S:2069:HOH:O	2.21	0.40
1:T:157:ASP:HB2	4:T:2104:HOH:O	2.04	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:SER:OG	1:S:203:LYS:CD[1_655]	1.44	0.76
1:D:274:LEU:CD1	1:M:253:ARG:NH2[5_555]	1.65	0.55
1:K:66:ALA:CB	1:S:199:GLN:NE2[1_655]	1.67	0.53
1:L:195:GLN:NE2	1:L:195:GLN:NE2[5_555]	1.75	0.45
1:K:98:ASP:N	1:S:203:LYS:NZ[1_655]	1.77	0.43
1:E:254:GLU:OE1	1:T:127:GLU:OE2[5_665]	1.98	0.22
1:K:97:SER:OG	1:S:203:LYS:CE[1_655]	2.01	0.19
1:K:66:ALA:CB	1:S:199:GLN:CD[1_655]	2.02	0.18
1:D:273:ALA:O	1:M:273:ALA:O[5_555]	2.05	0.15
1:K:66:ALA:CA	1:S:199:GLN:NE2[1_655]	2.08	0.12
1:H:155:GLU:OE2	1:T:270:SER:OG[5_665]	2.09	0.11
1:K:66:ALA:CB	1:S:199:GLN:OE1[1_655]	2.12	0.08
4:H:2043:HOH:O	4:R:2064:HOH:O[6_555]	2.16	0.04
1:T:274:LEU:CG	4:H:2169:HOH:O[5_565]	2.17	0.03
1:K:66:ALA:N	1:S:199:GLN:NE2[1_655]	2.18	0.02
1:L:195:GLN:CD	1:L:195:GLN:CD[5_555]	2.18	0.02
1:S:199:GLN:CG	4:K:2078:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	272/274 (99%)	264 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
1	C	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	D	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	E	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	F	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	G	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	H	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	I	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	J	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
1	K	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	L	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	M	272/274 (99%)	261 (96%)	11 (4%)	0	100	100
1	N	272/274 (99%)	263 (97%)	9 (3%)	0	100	100
1	O	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
1	P	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	Q	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	R	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	S	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
1	T	272/274 (99%)	262 (96%)	10 (4%)	0	100	100
All	All	5440/5480 (99%)	5259 (97%)	181 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	228/228 (100%)	203 (89%)	25 (11%)	6	15
1	B	228/228 (100%)	204 (90%)	24 (10%)	6	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	228/228 (100%)	203 (89%)	25 (11%)	6	15
1	D	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	E	228/228 (100%)	204 (90%)	24 (10%)	6	17
1	F	228/228 (100%)	204 (90%)	24 (10%)	6	17
1	G	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	H	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	I	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	J	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	K	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	L	228/228 (100%)	201 (88%)	27 (12%)	5	13
1	M	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	N	228/228 (100%)	201 (88%)	27 (12%)	5	13
1	O	228/228 (100%)	201 (88%)	27 (12%)	5	13
1	P	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	Q	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	R	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	S	228/228 (100%)	202 (89%)	26 (11%)	5	14
1	T	228/228 (100%)	204 (90%)	24 (10%)	6	17
All	All	4560/4560 (100%)	4047 (89%)	513 (11%)	5	14

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	32	ASN
1	A	33	LEU
1	A	52	GLN
1	A	58	LEU
1	A	84	LEU
1	A	108	LEU
1	A	135	LYS
1	A	137	ARG
1	A	147	LEU
1	A	153	VAL
1	A	160	VAL
1	A	161	PHE

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Mol	Chain	Res	Type
1	A	173	LEU
1	A	180	VAL
1	A	182	ILE
1	A	195	GLN
1	A	199	GLN
1	A	206	LEU
1	A	221	LEU
1	A	223	GLU
1	A	265	VAL
1	A	266	THR
1	A	272	LEU
1	A	274	LEU
1	B	32	ASN
1	B	33	LEU
1	B	52	GLN
1	B	58	LEU
1	B	84	LEU
1	B	108	LEU
1	B	135	LYS
1	B	137	ARG
1	B	147	LEU
1	B	153	VAL
1	B	160	VAL
1	B	161	PHE
1	B	173	LEU
1	B	180	VAL
1	B	182	ILE
1	B	195	GLN
1	B	199	GLN
1	B	206	LEU
1	B	221	LEU
1	B	248	LYS
1	B	265	VAL
1	B	266	THR
1	B	272	LEU
1	B	274	LEU
1	C	32	ASN
1	C	33	LEU
1	C	52	GLN
1	C	58	LEU
1	C	60	GLN
1	C	84	LEU

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Mol	Chain	Res	Type
1	C	108	LEU
1	C	135	LYS
1	C	137	ARG
1	C	147	LEU
1	C	153	VAL
1	C	160	VAL
1	C	161	PHE
1	C	173	LEU
1	C	180	VAL
1	C	182	ILE
1	C	195	GLN
1	C	199	GLN
1	C	206	LEU
1	C	221	LEU
1	C	223	GLU
1	C	265	VAL
1	C	266	THR
1	C	272	LEU
1	C	274	LEU
1	D	32	ASN
1	D	33	LEU
1	D	52	GLN
1	D	58	LEU
1	D	60	GLN
1	D	84	LEU
1	D	108	LEU
1	D	135	LYS
1	D	137	ARG
1	D	147	LEU
1	D	153	VAL
1	D	160	VAL
1	D	161	PHE
1	D	173	LEU
1	D	180	VAL
1	D	182	ILE
1	D	195	GLN
1	D	199	GLN
1	D	206	LEU
1	D	221	LEU
1	D	223	GLU
1	D	248	LYS
1	D	265	VAL

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Mol	Chain	Res	Type
1	D	266	THR
1	D	272	LEU
1	D	274	LEU
1	E	32	ASN
1	E	33	LEU
1	E	52	GLN
1	E	58	LEU
1	E	84	LEU
1	E	108	LEU
1	E	135	LYS
1	E	137	ARG
1	E	147	LEU
1	E	153	VAL
1	E	160	VAL
1	E	161	PHE
1	E	163	ARG
1	E	173	LEU
1	E	180	VAL
1	E	182	ILE
1	E	195	GLN
1	E	199	GLN
1	E	206	LEU
1	E	221	LEU
1	E	265	VAL
1	E	266	THR
1	E	272	LEU
1	E	274	LEU
1	F	32	ASN
1	F	33	LEU
1	F	52	GLN
1	F	58	LEU
1	F	84	LEU
1	F	108	LEU
1	F	135	LYS
1	F	137	ARG
1	F	147	LEU
1	F	153	VAL
1	F	160	VAL
1	F	161	PHE
1	F	173	LEU
1	F	180	VAL
1	F	182	ILE

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Mol	Chain	Res	Type
1	F	195	GLN
1	F	199	GLN
1	F	206	LEU
1	F	221	LEU
1	F	223	GLU
1	F	265	VAL
1	F	266	THR
1	F	272	LEU
1	F	274	LEU
1	G	32	ASN
1	G	33	LEU
1	G	52	GLN
1	G	58	LEU
1	G	84	LEU
1	G	108	LEU
1	G	135	LYS
1	G	137	ARG
1	G	147	LEU
1	G	153	VAL
1	G	160	VAL
1	G	161	PHE
1	G	163	ARG
1	G	173	LEU
1	G	180	VAL
1	G	182	ILE
1	G	195	GLN
1	G	199	GLN
1	G	206	LEU
1	G	221	LEU
1	G	223	GLU
1	G	248	LYS
1	G	265	VAL
1	G	266	THR
1	G	272	LEU
1	G	274	LEU
1	H	32	ASN
1	H	33	LEU
1	H	52	GLN
1	H	58	LEU
1	H	60	GLN
1	H	84	LEU
1	H	108	LEU

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Mol	Chain	Res	Type
1	H	135	LYS
1	H	137	ARG
1	H	147	LEU
1	H	153	VAL
1	H	160	VAL
1	H	161	PHE
1	H	163	ARG
1	H	173	LEU
1	H	180	VAL
1	H	182	ILE
1	H	195	GLN
1	H	199	GLN
1	H	206	LEU
1	H	221	LEU
1	H	223	GLU
1	H	265	VAL
1	H	266	THR
1	H	272	LEU
1	H	274	LEU
1	I	28	ARG
1	I	32	ASN
1	I	33	LEU
1	I	52	GLN
1	I	58	LEU
1	I	84	LEU
1	I	108	LEU
1	I	135	LYS
1	I	137	ARG
1	I	147	LEU
1	I	153	VAL
1	I	160	VAL
1	I	161	PHE
1	I	163	ARG
1	I	173	LEU
1	I	180	VAL
1	I	182	ILE
1	I	195	GLN
1	I	199	GLN
1	I	206	LEU
1	I	221	LEU
1	I	223	GLU
1	I	265	VAL

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Mol	Chain	Res	Type
1	I	266	THR
1	I	272	LEU
1	I	274	LEU
1	J	28	ARG
1	J	32	ASN
1	J	33	LEU
1	J	52	GLN
1	J	58	LEU
1	J	84	LEU
1	J	108	LEU
1	J	135	LYS
1	J	137	ARG
1	J	147	LEU
1	J	153	VAL
1	J	160	VAL
1	J	161	PHE
1	J	163	ARG
1	J	173	LEU
1	J	180	VAL
1	J	182	ILE
1	J	195	GLN
1	J	199	GLN
1	J	206	LEU
1	J	221	LEU
1	J	248	LYS
1	J	265	VAL
1	J	266	THR
1	J	272	LEU
1	J	274	LEU
1	K	32	ASN
1	K	33	LEU
1	K	52	GLN
1	K	58	LEU
1	K	84	LEU
1	K	108	LEU
1	K	135	LYS
1	K	137	ARG
1	K	147	LEU
1	K	153	VAL
1	K	160	VAL
1	K	161	PHE
1	K	163	ARG

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Mol	Chain	Res	Type
1	K	173	LEU
1	K	180	VAL
1	K	182	ILE
1	K	195	GLN
1	K	199	GLN
1	K	206	LEU
1	K	221	LEU
1	K	223	GLU
1	K	248	LYS
1	K	265	VAL
1	K	266	THR
1	K	272	LEU
1	K	274	LEU
1	L	28	ARG
1	L	32	ASN
1	L	33	LEU
1	L	52	GLN
1	L	58	LEU
1	L	84	LEU
1	L	108	LEU
1	L	135	LYS
1	L	137	ARG
1	L	147	LEU
1	L	153	VAL
1	L	160	VAL
1	L	161	PHE
1	L	163	ARG
1	L	173	LEU
1	L	180	VAL
1	L	182	ILE
1	L	195	GLN
1	L	199	GLN
1	L	206	LEU
1	L	221	LEU
1	L	223	GLU
1	L	248	LYS
1	L	265	VAL
1	L	266	THR
1	L	272	LEU
1	L	274	LEU
1	M	28	ARG
1	M	32	ASN

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Mol	Chain	Res	Type
1	M	33	LEU
1	M	52	GLN
1	M	58	LEU
1	M	84	LEU
1	M	108	LEU
1	M	135	LYS
1	M	137	ARG
1	M	147	LEU
1	M	153	VAL
1	M	160	VAL
1	M	161	PHE
1	M	163	ARG
1	M	173	LEU
1	M	180	VAL
1	M	182	ILE
1	M	195	GLN
1	M	199	GLN
1	M	206	LEU
1	M	221	LEU
1	M	248	LYS
1	M	265	VAL
1	M	266	THR
1	M	272	LEU
1	M	274	LEU
1	N	32	ASN
1	N	33	LEU
1	N	52	GLN
1	N	58	LEU
1	N	84	LEU
1	N	108	LEU
1	N	135	LYS
1	N	137	ARG
1	N	147	LEU
1	N	153	VAL
1	N	160	VAL
1	N	161	PHE
1	N	163	ARG
1	N	173	LEU
1	N	180	VAL
1	N	182	ILE
1	N	195	GLN
1	N	199	GLN

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Mol	Chain	Res	Type
1	N	203	LYS
1	N	206	LEU
1	N	221	LEU
1	N	223	GLU
1	N	248	LYS
1	N	265	VAL
1	N	266	THR
1	N	272	LEU
1	N	274	LEU
1	O	32	ASN
1	O	33	LEU
1	O	52	GLN
1	O	58	LEU
1	O	60	GLN
1	O	84	LEU
1	O	108	LEU
1	O	135	LYS
1	O	137	ARG
1	O	147	LEU
1	O	153	VAL
1	O	160	VAL
1	O	161	PHE
1	O	163	ARG
1	O	173	LEU
1	O	180	VAL
1	O	182	ILE
1	O	195	GLN
1	O	199	GLN
1	O	206	LEU
1	O	221	LEU
1	O	223	GLU
1	O	248	LYS
1	O	265	VAL
1	O	266	THR
1	O	272	LEU
1	O	274	LEU
1	P	32	ASN
1	P	33	LEU
1	P	52	GLN
1	P	58	LEU
1	P	84	LEU
1	P	108	LEU

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Mol	Chain	Res	Type
1	P	135	LYS
1	P	137	ARG
1	P	147	LEU
1	P	153	VAL
1	P	160	VAL
1	P	161	PHE
1	P	163	ARG
1	P	173	LEU
1	P	180	VAL
1	P	182	ILE
1	P	195	GLN
1	P	199	GLN
1	P	206	LEU
1	P	221	LEU
1	P	223	GLU
1	P	248	LYS
1	P	265	VAL
1	P	266	THR
1	P	272	LEU
1	P	274	LEU
1	Q	32	ASN
1	Q	33	LEU
1	Q	52	GLN
1	Q	58	LEU
1	Q	84	LEU
1	Q	108	LEU
1	Q	135	LYS
1	Q	137	ARG
1	Q	147	LEU
1	Q	153	VAL
1	Q	160	VAL
1	Q	161	PHE
1	Q	163	ARG
1	Q	173	LEU
1	Q	180	VAL
1	Q	182	ILE
1	Q	195	GLN
1	Q	199	GLN
1	Q	206	LEU
1	Q	221	LEU
1	Q	223	GLU
1	Q	248	LYS

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Mol	Chain	Res	Type
1	Q	265	VAL
1	Q	266	THR
1	Q	272	LEU
1	Q	274	LEU
1	R	28	ARG
1	R	32	ASN
1	R	33	LEU
1	R	52	GLN
1	R	58	LEU
1	R	84	LEU
1	R	108	LEU
1	R	135	LYS
1	R	137	ARG
1	R	147	LEU
1	R	153	VAL
1	R	160	VAL
1	R	161	PHE
1	R	173	LEU
1	R	180	VAL
1	R	182	ILE
1	R	195	GLN
1	R	199	GLN
1	R	206	LEU
1	R	221	LEU
1	R	223	GLU
1	R	248	LYS
1	R	265	VAL
1	R	266	THR
1	R	272	LEU
1	R	274	LEU
1	S	32	ASN
1	S	33	LEU
1	S	52	GLN
1	S	58	LEU
1	S	84	LEU
1	S	108	LEU
1	S	135	LYS
1	S	137	ARG
1	S	147	LEU
1	S	153	VAL
1	S	160	VAL
1	S	161	PHE

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Mol	Chain	Res	Type
1	S	163	ARG
1	S	164	GLN
1	S	173	LEU
1	S	180	VAL
1	S	182	ILE
1	S	195	GLN
1	S	199	GLN
1	S	206	LEU
1	S	221	LEU
1	S	223	GLU
1	S	265	VAL
1	S	266	THR
1	S	272	LEU
1	S	274	LEU
1	T	32	ASN
1	T	33	LEU
1	T	52	GLN
1	T	58	LEU
1	T	84	LEU
1	T	108	LEU
1	T	135	LYS
1	T	147	LEU
1	T	153	VAL
1	T	160	VAL
1	T	161	PHE
1	T	163	ARG
1	T	173	LEU
1	T	180	VAL
1	T	182	ILE
1	T	195	GLN
1	T	199	GLN
1	T	206	LEU
1	T	221	LEU
1	T	223	GLU
1	T	265	VAL
1	T	266	THR
1	T	272	LEU
1	T	274	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	156	ASN
1	A	164	GLN
1	A	195	GLN
1	A	204	HIS
1	B	60	GLN
1	B	156	ASN
1	B	164	GLN
1	B	195	GLN
1	B	204	HIS
1	C	60	GLN
1	C	156	ASN
1	C	164	GLN
1	C	195	GLN
1	C	204	HIS
1	D	6	GLN
1	D	50	HIS
1	D	60	GLN
1	D	156	ASN
1	D	195	GLN
1	D	204	HIS
1	E	6	GLN
1	E	50	HIS
1	E	60	GLN
1	E	156	ASN
1	E	164	GLN
1	E	195	GLN
1	E	204	HIS
1	F	46	HIS
1	F	60	GLN
1	F	156	ASN
1	F	195	GLN
1	F	204	HIS
1	G	6	GLN
1	G	60	GLN
1	G	156	ASN
1	G	164	GLN
1	G	195	GLN
1	G	204	HIS
1	H	50	HIS
1	H	60	GLN
1	H	156	ASN
1	H	195	GLN

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Mol	Chain	Res	Type
1	H	204	HIS
1	I	60	GLN
1	I	156	ASN
1	I	164	GLN
1	I	195	GLN
1	I	204	HIS
1	J	6	GLN
1	J	50	HIS
1	J	60	GLN
1	J	156	ASN
1	J	164	GLN
1	J	195	GLN
1	J	204	HIS
1	K	60	GLN
1	K	156	ASN
1	K	164	GLN
1	K	195	GLN
1	K	204	HIS
1	L	50	HIS
1	L	60	GLN
1	L	156	ASN
1	L	164	GLN
1	L	195	GLN
1	L	204	HIS
1	M	6	GLN
1	M	60	GLN
1	M	110	ASN
1	M	156	ASN
1	M	164	GLN
1	M	195	GLN
1	M	204	HIS
1	N	6	GLN
1	N	50	HIS
1	N	60	GLN
1	N	156	ASN
1	N	164	GLN
1	N	195	GLN
1	N	204	HIS
1	O	6	GLN
1	O	50	HIS
1	O	60	GLN
1	O	156	ASN

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Mol	Chain	Res	Type
1	O	195	GLN
1	O	204	HIS
1	P	50	HIS
1	P	60	GLN
1	P	156	ASN
1	P	164	GLN
1	P	195	GLN
1	P	204	HIS
1	Q	60	GLN
1	Q	156	ASN
1	Q	164	GLN
1	Q	195	GLN
1	Q	204	HIS
1	R	50	HIS
1	R	60	GLN
1	R	156	ASN
1	R	164	GLN
1	R	195	GLN
1	R	204	HIS
1	S	46	HIS
1	S	50	HIS
1	S	60	GLN
1	S	156	ASN
1	S	164	GLN
1	S	195	GLN
1	S	204	HIS
1	T	6	GLN
1	T	50	HIS
1	T	60	GLN
1	T	156	ASN
1	T	164	GLN
1	T	195	GLN
1	T	204	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 20 are monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PGH	R	300	2	9,9,9	3.09	5 (55%)	10,12,12	2.08	4 (40%)
3	PGH	G	300	2	9,9,9	3.20	6 (66%)	10,12,12	2.14	3 (30%)
3	PGH	S	300	2	9,9,9	2.94	5 (55%)	10,12,12	2.06	3 (30%)
3	PGH	O	300	2	9,9,9	3.59	5 (55%)	10,12,12	2.90	5 (50%)
3	PGH	J	300	2	9,9,9	3.48	5 (55%)	10,12,12	2.94	6 (60%)
3	PGH	B	300	2	9,9,9	3.08	5 (55%)	10,12,12	2.65	5 (50%)
3	PGH	C	300	2	9,9,9	3.33	5 (55%)	10,12,12	2.14	6 (60%)
3	PGH	F	300	2	9,9,9	2.85	5 (55%)	10,12,12	2.52	3 (30%)
3	PGH	A	300	2	9,9,9	3.06	5 (55%)	10,12,12	2.17	4 (40%)
3	PGH	H	300	2	9,9,9	3.30	6 (66%)	10,12,12	2.14	5 (50%)
3	PGH	P	300	2	9,9,9	3.41	5 (55%)	10,12,12	2.42	3 (30%)
3	PGH	Q	300	2	9,9,9	3.26	5 (55%)	10,12,12	2.45	4 (40%)
3	PGH	N	300	2	9,9,9	3.18	5 (55%)	10,12,12	2.91	3 (30%)
3	PGH	T	300	2	9,9,9	3.35	7 (77%)	10,12,12	2.09	5 (50%)
3	PGH	L	300	2	9,9,9	3.71	5 (55%)	10,12,12	2.60	4 (40%)
3	PGH	D	300	2	9,9,9	3.29	5 (55%)	10,12,12	2.40	4 (40%)
3	PGH	I	300	2	9,9,9	3.01	4 (44%)	10,12,12	2.92	3 (30%)
3	PGH	M	300	2	9,9,9	3.64	5 (55%)	10,12,12	2.73	4 (40%)
3	PGH	E	300	2	9,9,9	3.21	4 (44%)	10,12,12	2.86	6 (60%)
3	PGH	K	300	2	9,9,9	3.30	5 (55%)	10,12,12	2.93	4 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGH	R	300	2	-	5/8/8/8	-
3	PGH	G	300	2	-	4/8/8/8	-
3	PGH	S	300	2	-	5/8/8/8	-
3	PGH	O	300	2	-	5/8/8/8	-
3	PGH	J	300	2	-	5/8/8/8	-
3	PGH	B	300	2	-	5/8/8/8	-
3	PGH	C	300	2	-	5/8/8/8	-
3	PGH	F	300	2	-	5/8/8/8	-
3	PGH	A	300	2	-	5/8/8/8	-
3	PGH	H	300	2	-	5/8/8/8	-
3	PGH	P	300	2	-	5/8/8/8	-
3	PGH	Q	300	2	-	3/8/8/8	-
3	PGH	N	300	2	-	3/8/8/8	-
3	PGH	T	300	2	-	5/8/8/8	-
3	PGH	L	300	2	-	5/8/8/8	-
3	PGH	D	300	2	-	5/8/8/8	-
3	PGH	I	300	2	-	5/8/8/8	-
3	PGH	M	300	2	-	5/8/8/8	-
3	PGH	E	300	2	-	5/8/8/8	-
3	PGH	K	300	2	-	5/8/8/8	-

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	300	PGH	P-O1P	7.24	1.83	1.60
3	C	300	PGH	P-O1P	7.13	1.82	1.60
3	D	300	PGH	P-O1P	6.63	1.81	1.60
3	A	300	PGH	P-O1P	6.59	1.81	1.60
3	E	300	PGH	P-O1P	6.47	1.80	1.60
3	P	300	PGH	P-O1P	6.38	1.80	1.60
3	Q	300	PGH	P-O1P	6.37	1.80	1.60
3	H	300	PGH	P-O1P	6.31	1.80	1.60
3	B	300	PGH	P-O1P	6.02	1.79	1.60
3	L	300	PGH	P-O1P	5.97	1.79	1.60
3	J	300	PGH	P-O1P	5.91	1.79	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	300	PGH	P-O1P	5.89	1.78	1.60
3	K	300	PGH	P-O1P	5.78	1.78	1.60
3	L	300	PGH	O1P-C2	-5.65	1.37	1.43
3	O	300	PGH	P-O1P	5.55	1.77	1.60
3	G	300	PGH	P-O1P	5.41	1.77	1.60
3	O	300	PGH	O1P-C2	-5.30	1.38	1.43
3	S	300	PGH	P-O1P	5.28	1.77	1.60
3	T	300	PGH	P-O1P	5.27	1.76	1.60
3	R	300	PGH	P-O1P	5.26	1.76	1.60
3	I	300	PGH	P-O1P	5.19	1.76	1.60
3	J	300	PGH	P-O2P	5.16	1.66	1.50
3	L	300	PGH	P-O4P	4.96	1.73	1.54
3	T	300	PGH	O1P-C2	-4.86	1.38	1.43
3	O	300	PGH	P-O4P	4.85	1.72	1.54
3	P	300	PGH	P-O2P	4.78	1.65	1.50
3	F	300	PGH	P-O1P	4.73	1.75	1.60
3	D	300	PGH	O1P-C2	-4.64	1.38	1.43
3	E	300	PGH	P-O2P	4.53	1.64	1.50
3	M	300	PGH	O1P-C2	-4.50	1.38	1.43
3	I	300	PGH	P-O2P	4.49	1.64	1.50
3	I	300	PGH	P-O4P	4.47	1.71	1.54
3	O	300	PGH	P-O2P	4.45	1.64	1.50
3	N	300	PGH	P-O2P	4.44	1.64	1.50
3	R	300	PGH	O1P-C2	-4.43	1.39	1.43
3	M	300	PGH	P-O2P	4.42	1.64	1.50
3	E	300	PGH	P-O4P	4.36	1.71	1.54
3	M	300	PGH	P-O4P	4.34	1.70	1.54
3	J	300	PGH	O1P-C2	-4.33	1.39	1.43
3	H	300	PGH	O1P-C2	-4.33	1.39	1.43
3	L	300	PGH	P-O2P	4.30	1.63	1.50
3	K	300	PGH	P-O2P	4.24	1.63	1.50
3	F	300	PGH	P-O2P	4.23	1.63	1.50
3	N	300	PGH	P-O4P	4.23	1.70	1.54
3	G	300	PGH	O1P-C2	-4.23	1.39	1.43
3	Q	300	PGH	P-O2P	4.22	1.63	1.50
3	K	300	PGH	P-O4P	4.20	1.70	1.54
3	B	300	PGH	P-O2P	4.19	1.63	1.50
3	S	300	PGH	P-O2P	4.11	1.63	1.50
3	R	300	PGH	P-O2P	4.11	1.63	1.50
3	C	300	PGH	P-O2P	4.03	1.63	1.50
3	Q	300	PGH	P-O4P	4.02	1.69	1.54
3	K	300	PGH	O1P-C2	-4.01	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	300	PGH	P-O4P	3.99	1.69	1.54
3	D	300	PGH	P-O4P	3.92	1.69	1.54
3	C	300	PGH	P-O4P	3.92	1.69	1.54
3	F	300	PGH	P-O4P	3.89	1.69	1.54
3	T	300	PGH	P-O4P	3.83	1.69	1.54
3	J	300	PGH	P-O4P	3.82	1.69	1.54
3	H	300	PGH	P-O4P	3.80	1.68	1.54
3	P	300	PGH	P-O3P	3.75	1.68	1.54
3	A	300	PGH	P-O2P	3.71	1.62	1.50
3	P	300	PGH	P-O4P	3.68	1.68	1.54
3	H	300	PGH	P-O2P	3.65	1.61	1.50
3	B	300	PGH	O1P-C2	-3.59	1.39	1.43
3	T	300	PGH	P-O2P	3.52	1.61	1.50
3	Q	300	PGH	O1P-C2	-3.51	1.39	1.43
3	S	300	PGH	P-O4P	3.50	1.67	1.54
3	O	300	PGH	P-O3P	3.37	1.67	1.54
3	D	300	PGH	P-O2P	3.34	1.60	1.50
3	T	300	PGH	P-O3P	3.32	1.67	1.54
3	B	300	PGH	P-O4P	3.29	1.67	1.54
3	L	300	PGH	P-O3P	3.19	1.66	1.54
3	N	300	PGH	P-O3P	3.15	1.66	1.54
3	R	300	PGH	P-O4P	3.11	1.66	1.54
3	J	300	PGH	P-O3P	3.10	1.66	1.54
3	G	300	PGH	P-O3P	3.08	1.66	1.54
3	K	300	PGH	P-O3P	3.06	1.66	1.54
3	G	300	PGH	P-O2P	3.02	1.59	1.50
3	I	300	PGH	P-O3P	3.01	1.66	1.54
3	R	300	PGH	P-O3P	3.00	1.65	1.54
3	A	300	PGH	P-O4P	2.90	1.65	1.54
3	F	300	PGH	P-O3P	2.88	1.65	1.54
3	S	300	PGH	P-O3P	2.86	1.65	1.54
3	A	300	PGH	P-O3P	2.85	1.65	1.54
3	N	300	PGH	O1P-C2	-2.75	1.40	1.43
3	S	300	PGH	O1P-C2	-2.74	1.40	1.43
3	C	300	PGH	O1P-C2	-2.70	1.40	1.43
3	F	300	PGH	O1P-C2	-2.69	1.40	1.43
3	G	300	PGH	C1-N2	-2.57	1.29	1.32
3	P	300	PGH	O1P-C2	-2.50	1.40	1.43
3	C	300	PGH	P-O3P	2.46	1.64	1.54
3	A	300	PGH	O1P-C2	-2.46	1.40	1.43
3	E	300	PGH	P-O3P	2.36	1.63	1.54
3	T	300	PGH	C1-N2	-2.33	1.29	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	300	PGH	P-O3P	2.26	1.63	1.54
3	M	300	PGH	P-O3P	2.24	1.63	1.54
3	Q	300	PGH	P-O3P	2.17	1.62	1.54
3	T	300	PGH	O2-N2	-2.16	1.34	1.40
3	B	300	PGH	P-O3P	2.14	1.62	1.54
3	H	300	PGH	O2-N2	-2.10	1.34	1.40
3	D	300	PGH	P-O3P	2.05	1.62	1.54

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	300	PGH	O1-C1-N2	6.34	131.06	123.27
3	J	300	PGH	O1-C1-N2	6.32	131.03	123.27
3	N	300	PGH	O1-C1-N2	6.31	131.02	123.27
3	I	300	PGH	O1-C1-N2	6.12	130.78	123.27
3	K	300	PGH	O1-C1-N2	6.06	130.71	123.27
3	E	300	PGH	O1-C1-N2	5.89	130.50	123.27
3	M	300	PGH	O1-C1-N2	5.84	130.44	123.27
3	I	300	PGH	O3P-P-O1P	5.06	119.86	106.67
3	B	300	PGH	O1-C1-N2	4.87	129.25	123.27
3	K	300	PGH	O3P-P-O1P	4.83	119.26	106.67
3	F	300	PGH	O1-C1-N2	4.80	129.17	123.27
3	L	300	PGH	O1-C1-N2	4.79	129.15	123.27
3	O	300	PGH	O3P-P-O1P	4.50	118.40	106.67
3	P	300	PGH	O1-C1-N2	4.50	128.79	123.27
3	F	300	PGH	O3P-P-O1P	4.47	118.34	106.67
3	N	300	PGH	O3P-P-O1P	4.46	118.30	106.67
3	D	300	PGH	O1-C1-N2	4.42	128.70	123.27
3	P	300	PGH	O3P-P-O1P	4.39	118.11	106.67
3	S	300	PGH	O3P-P-O1P	4.37	118.07	106.67
3	L	300	PGH	O3P-P-O1P	4.33	117.95	106.67
3	B	300	PGH	O3P-P-O1P	4.09	117.32	106.67
3	J	300	PGH	O3P-P-O1P	4.09	117.32	106.67
3	E	300	PGH	O3P-P-O1P	4.01	117.14	106.67
3	Q	300	PGH	O3P-P-O1P	3.96	117.00	106.67
3	T	300	PGH	O3P-P-O1P	3.87	116.75	106.67
3	A	300	PGH	O1-C1-N2	3.80	127.94	123.27
3	Q	300	PGH	O1-C1-N2	3.80	127.93	123.27
3	R	300	PGH	O3P-P-O1P	3.77	116.51	106.67
3	G	300	PGH	O3P-P-O1P	3.67	116.23	106.67
3	Q	300	PGH	O4P-P-O1P	-3.50	97.54	106.67
3	H	300	PGH	O3P-P-O1P	3.48	115.74	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	300	PGH	O3P-P-O1P	3.42	115.58	106.67
3	G	300	PGH	O1-C1-N2	3.41	127.46	123.27
3	A	300	PGH	O3P-P-O1P	3.19	115.00	106.67
3	H	300	PGH	O4P-P-O1P	-3.19	98.36	106.67
3	R	300	PGH	O1-C1-N2	3.18	127.17	123.27
3	D	300	PGH	O3P-P-O1P	3.17	114.94	106.67
3	C	300	PGH	O3P-P-O1P	3.10	114.74	106.67
3	D	300	PGH	O4P-P-O1P	-3.09	98.61	106.67
3	B	300	PGH	O4P-P-O1P	-3.01	98.81	106.67
3	C	300	PGH	O1-C1-N2	2.99	126.94	123.27
3	I	300	PGH	O4P-P-O1P	-2.98	98.90	106.67
3	K	300	PGH	O4P-P-O1P	-2.98	98.90	106.67
3	S	300	PGH	O1-C1-N2	2.96	126.90	123.27
3	E	300	PGH	O4P-P-O1P	-2.87	99.19	106.67
3	N	300	PGH	O4P-P-O1P	-2.86	99.22	106.67
3	C	300	PGH	O1P-P-O2P	-2.86	98.71	106.44
3	M	300	PGH	O4P-P-O1P	-2.80	99.36	106.67
3	T	300	PGH	O1-C1-N2	2.71	126.60	123.27
3	F	300	PGH	O4P-P-O1P	-2.69	99.65	106.67
3	P	300	PGH	O4P-P-O1P	-2.66	99.72	106.67
3	H	300	PGH	O3P-P-O2P	2.65	121.15	110.83
3	L	300	PGH	O4P-P-O1P	-2.61	99.87	106.67
3	B	300	PGH	O1P-P-O2P	-2.58	99.47	106.44
3	R	300	PGH	O4P-P-O1P	-2.52	100.10	106.67
3	D	300	PGH	O3P-P-O2P	2.49	120.53	110.83
3	J	300	PGH	O4P-P-O1P	-2.44	100.32	106.67
3	A	300	PGH	O4P-P-O1P	-2.42	100.36	106.67
3	B	300	PGH	O4P-P-O3P	2.41	116.86	107.80
3	M	300	PGH	O4P-P-O3P	2.41	116.85	107.80
3	A	300	PGH	O1P-P-O2P	-2.39	99.98	106.44
3	E	300	PGH	O3P-P-O2P	2.38	120.12	110.83
3	G	300	PGH	O4P-P-O1P	-2.36	100.52	106.67
3	C	300	PGH	O4P-P-O1P	-2.35	100.55	106.67
3	C	300	PGH	O3P-P-O2P	2.30	119.78	110.83
3	L	300	PGH	O2-N2-C1	2.28	123.16	119.79
3	O	300	PGH	O1P-P-O2P	-2.26	100.34	106.44
3	T	300	PGH	O1P-P-O2P	-2.25	100.37	106.44
3	O	300	PGH	O3P-P-O2P	2.22	119.48	110.83
3	E	300	PGH	O4P-P-O2P	-2.21	102.22	110.83
3	H	300	PGH	O1-C1-N2	2.21	125.98	123.27
3	E	300	PGH	O1P-P-O2P	-2.19	100.51	106.44
3	S	300	PGH	O4P-P-O1P	-2.19	100.95	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	300	PGH	O4P-P-O2P	-2.18	102.34	110.83
3	O	300	PGH	O4P-P-O1P	-2.18	101.00	106.67
3	J	300	PGH	O1P-P-O2P	-2.17	100.58	106.44
3	T	300	PGH	O3P-P-O2P	2.17	119.28	110.83
3	H	300	PGH	O1P-P-O2P	-2.17	100.59	106.44
3	J	300	PGH	O4P-P-O3P	2.15	115.85	107.80
3	Q	300	PGH	O4P-P-O3P	2.14	115.82	107.80
3	K	300	PGH	O1P-P-O2P	-2.10	100.75	106.44
3	R	300	PGH	O4P-P-O3P	2.05	115.49	107.80
3	T	300	PGH	O4P-P-O2P	-2.04	102.87	110.83
3	C	300	PGH	O4P-P-O3P	2.02	115.37	107.80

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	300	PGH	N2-C1-C2-O1P
3	A	300	PGH	C2-O1P-P-O4P
3	B	300	PGH	N2-C1-C2-O1P
3	B	300	PGH	C2-O1P-P-O3P
3	B	300	PGH	C2-O1P-P-O4P
3	C	300	PGH	N2-C1-C2-O1P
3	C	300	PGH	C2-O1P-P-O3P
3	C	300	PGH	C2-O1P-P-O4P
3	D	300	PGH	N2-C1-C2-O1P
3	D	300	PGH	C2-O1P-P-O4P
3	E	300	PGH	N2-C1-C2-O1P
3	E	300	PGH	C2-O1P-P-O4P
3	F	300	PGH	C2-O1P-P-O4P
3	G	300	PGH	C2-O1P-P-O4P
3	H	300	PGH	N2-C1-C2-O1P
3	H	300	PGH	C2-O1P-P-O4P
3	I	300	PGH	N2-C1-C2-O1P
3	I	300	PGH	C2-O1P-P-O4P
3	J	300	PGH	N2-C1-C2-O1P
3	J	300	PGH	C2-O1P-P-O3P
3	J	300	PGH	C2-O1P-P-O4P
3	K	300	PGH	N2-C1-C2-O1P
3	K	300	PGH	C2-O1P-P-O4P
3	L	300	PGH	C2-O1P-P-O4P
3	M	300	PGH	N2-C1-C2-O1P
3	M	300	PGH	C2-O1P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	M	300	PGH	C2-O1P-P-O4P
3	N	300	PGH	C2-O1P-P-O4P
3	O	300	PGH	N2-C1-C2-O1P
3	O	300	PGH	C2-O1P-P-O4P
3	P	300	PGH	N2-C1-C2-O1P
3	P	300	PGH	C2-O1P-P-O4P
3	Q	300	PGH	C2-O1P-P-O4P
3	R	300	PGH	N2-C1-C2-O1P
3	R	300	PGH	C2-O1P-P-O3P
3	R	300	PGH	C2-O1P-P-O4P
3	S	300	PGH	N2-C1-C2-O1P
3	S	300	PGH	C2-O1P-P-O3P
3	S	300	PGH	C2-O1P-P-O4P
3	T	300	PGH	C2-O1P-P-O4P
3	A	300	PGH	C2-O1P-P-O2P
3	B	300	PGH	C2-O1P-P-O2P
3	C	300	PGH	C2-O1P-P-O2P
3	D	300	PGH	C2-O1P-P-O2P
3	E	300	PGH	C2-O1P-P-O2P
3	F	300	PGH	C2-O1P-P-O2P
3	G	300	PGH	C2-O1P-P-O2P
3	H	300	PGH	C2-O1P-P-O2P
3	I	300	PGH	C2-O1P-P-O2P
3	J	300	PGH	C2-O1P-P-O2P
3	K	300	PGH	C2-O1P-P-O2P
3	L	300	PGH	C2-O1P-P-O2P
3	M	300	PGH	C2-O1P-P-O2P
3	N	300	PGH	C2-O1P-P-O2P
3	O	300	PGH	C2-O1P-P-O2P
3	P	300	PGH	C2-O1P-P-O2P
3	Q	300	PGH	C2-O1P-P-O2P
3	R	300	PGH	C2-O1P-P-O2P
3	S	300	PGH	C2-O1P-P-O2P
3	T	300	PGH	C2-O1P-P-O2P
3	K	300	PGH	O1-C1-C2-O1P
3	A	300	PGH	C2-O1P-P-O3P
3	E	300	PGH	C2-O1P-P-O3P
3	F	300	PGH	C2-O1P-P-O3P
3	G	300	PGH	C2-O1P-P-O3P
3	H	300	PGH	C2-O1P-P-O3P
3	I	300	PGH	C2-O1P-P-O3P
3	K	300	PGH	C2-O1P-P-O3P

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Mol	Chain	Res	Type	Atoms
3	L	300	PGH	C2-O1P-P-O3P
3	O	300	PGH	C2-O1P-P-O3P
3	P	300	PGH	C2-O1P-P-O3P
3	Q	300	PGH	C2-O1P-P-O3P
3	T	300	PGH	C2-O1P-P-O3P
3	C	300	PGH	O1-C1-C2-O1P
3	A	300	PGH	O1-C1-C2-O1P
3	D	300	PGH	O1-C1-C2-O1P
3	H	300	PGH	O1-C1-C2-O1P
3	I	300	PGH	O1-C1-C2-O1P
3	M	300	PGH	O1-C1-C2-O1P
3	S	300	PGH	O1-C1-C2-O1P
3	F	300	PGH	N2-C1-C2-O1P
3	L	300	PGH	N2-C1-C2-O1P
3	T	300	PGH	N2-C1-C2-O1P
3	B	300	PGH	O1-C1-C2-O1P
3	O	300	PGH	O1-C1-C2-O1P
3	P	300	PGH	O1-C1-C2-O1P
3	R	300	PGH	O1-C1-C2-O1P
3	E	300	PGH	O1-C1-C2-O1P
3	J	300	PGH	O1-C1-C2-O1P
3	G	300	PGH	O1-C1-C2-O1P
3	T	300	PGH	O1-C1-C2-O1P
3	L	300	PGH	O1-C1-C2-O1P
3	D	300	PGH	C2-O1P-P-O3P
3	N	300	PGH	C2-O1P-P-O3P
3	F	300	PGH	O1-C1-C2-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	300	PGH	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	274/274 (100%)	0.33	10 (3%)	46	42	23, 37, 60, 84	0
1	B	274/274 (100%)	0.27	12 (4%)	39	35	23, 37, 60, 84	0
1	C	274/274 (100%)	0.27	9 (3%)	49	45	23, 37, 60, 84	0
1	D	274/274 (100%)	0.49	20 (7%)	21	18	23, 37, 60, 84	0
1	E	274/274 (100%)	0.24	10 (3%)	46	42	23, 37, 60, 84	0
1	F	274/274 (100%)	0.08	2 (0%)	84	83	23, 37, 60, 84	0
1	G	274/274 (100%)	0.11	3 (1%)	78	76	23, 37, 60, 84	0
1	H	274/274 (100%)	0.41	22 (8%)	18	15	23, 37, 60, 84	0
1	I	274/274 (100%)	0.34	7 (2%)	57	54	23, 37, 60, 84	0
1	J	274/274 (100%)	0.39	6 (2%)	62	59	23, 37, 60, 84	0
1	K	274/274 (100%)	0.84	13 (4%)	36	33	23, 37, 60, 84	0
1	L	274/274 (100%)	0.75	10 (3%)	46	42	23, 37, 60, 84	0
1	M	274/274 (100%)	0.25	12 (4%)	39	35	23, 37, 60, 84	0
1	N	274/274 (100%)	0.30	3 (1%)	78	76	23, 37, 60, 84	0
1	O	274/274 (100%)	0.81	16 (5%)	29	25	23, 37, 60, 84	0
1	P	274/274 (100%)	0.59	10 (3%)	46	42	23, 37, 60, 84	0
1	Q	274/274 (100%)	0.46	15 (5%)	30	27	23, 37, 60, 84	0
1	R	274/274 (100%)	0.20	6 (2%)	62	59	23, 37, 60, 84	0
1	S	274/274 (100%)	0.24	7 (2%)	57	54	23, 37, 60, 84	0
1	T	274/274 (100%)	0.25	7 (2%)	57	54	23, 37, 60, 84	0
All	All	5480/5480 (100%)	0.38	200 (3%)	46	42	23, 37, 60, 84	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	51	GLN	7.7
1	D	51	GLN	6.7
1	Q	51	GLN	6.6
1	M	273	ALA	6.5
1	M	274	LEU	6.3
1	D	273	ALA	6.2
1	D	52	GLN	5.7
1	S	203	LYS	5.6
1	D	274	LEU	5.5
1	Q	52	GLN	5.3
1	C	51	GLN	5.2
1	A	52	GLN	5.2
1	I	51	GLN	5.1
1	S	199	GLN	5.1
1	Q	254	GLU	5.0
1	H	63	PRO	4.9
1	M	52	GLN	4.9
1	D	253	ARG	4.8
1	C	52	GLN	4.7
1	H	52	GLN	4.7
1	B	51	GLN	4.7
1	H	155	GLU	4.7
1	D	272	LEU	4.6
1	M	51	GLN	4.6
1	M	272	LEU	4.5
1	M	253	ARG	4.4
1	E	51	GLN	4.3
1	K	63	PRO	4.3
1	I	52	GLN	4.2
1	M	53	PRO	4.1
1	D	53	PRO	4.0
1	Q	50	HIS	4.0
1	M	64	LEU	4.0
1	Q	53	PRO	4.0
1	H	203	LYS	4.0
1	D	50	HIS	3.9
1	L	61	PRO	3.8
1	R	52	GLN	3.8
1	E	53	PRO	3.8
1	E	52	GLN	3.8
1	L	52	GLN	3.7
1	M	50	HIS	3.7
1	A	50	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	O	64	LEU	3.5
1	K	97	SER	3.5
1	Q	248	LYS	3.5
1	B	52	GLN	3.5
1	E	254	GLU	3.4
1	H	61	PRO	3.4
1	I	53	PRO	3.4
1	A	64	LEU	3.3
1	S	52	GLN	3.3
1	S	51	GLN	3.2
1	M	111	GLU	3.2
1	O	63	PRO	3.2
1	E	64	LEU	3.1
1	D	262	ARG	3.1
1	A	49	PHE	3.1
1	I	50	HIS	3.1
1	O	51	GLN	3.1
1	I	64	LEU	3.0
1	H	59	SER	3.0
1	H	191	ASP	3.0
1	R	262	ARG	3.0
1	L	64	LEU	3.0
1	Q	64	LEU	3.0
1	Q	133	ASN	3.0
1	A	53	PRO	2.9
1	K	59	SER	2.9
1	R	53	PRO	2.9
1	Q	49	PHE	2.9
1	B	64	LEU	2.9
1	H	64	LEU	2.9
1	E	50	HIS	2.9
1	O	266	THR	2.9
1	D	133	ASN	2.9
1	N	64	LEU	2.9
1	T	51	GLN	2.9
1	Q	60	GLN	2.8
1	E	49	PHE	2.8
1	P	64	LEU	2.8
1	O	100	ALA	2.8
1	H	199	GLN	2.8
1	O	52	GLN	2.8
1	B	59	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	111	GLU	2.8
1	H	126	CYS	2.7
1	B	53	PRO	2.7
1	K	61	PRO	2.7
1	R	261	LYS	2.7
1	B	50	HIS	2.7
1	H	100	ALA	2.7
1	K	51	GLN	2.7
1	C	50	HIS	2.7
1	O	273	ALA	2.7
1	K	52	GLN	2.6
1	S	202	GLN	2.6
1	D	64	LEU	2.6
1	H	99	GLY	2.6
1	L	63	PRO	2.6
1	F	262	ARG	2.6
1	D	261	LYS	2.6
1	J	135	LYS	2.6
1	C	59	SER	2.5
1	D	47	ASP	2.5
1	H	135	LYS	2.5
1	K	187	VAL	2.5
1	I	49	PHE	2.5
1	J	51	GLN	2.5
1	K	66	ALA	2.5
1	B	135	LYS	2.5
1	O	58	LEU	2.5
1	N	52	GLN	2.5
1	J	64	LEU	2.5
1	H	60	GLN	2.5
1	H	62	MET	2.5
1	C	133	ASN	2.5
1	B	192	GLU	2.5
1	F	52	GLN	2.5
1	P	58	LEU	2.4
1	A	192	GLU	2.4
1	C	223	GLU	2.4
1	D	49	PHE	2.4
1	H	58	LEU	2.4
1	P	97	SER	2.4
1	P	135	LYS	2.4
1	G	52	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	157	ASP	2.3
1	K	98	ASP	2.3
1	H	195	GLN	2.3
1	P	52	GLN	2.3
1	T	199	GLN	2.3
1	C	192	GLU	2.3
1	B	98	ASP	2.3
1	E	47	ASP	2.3
1	L	51	GLN	2.3
1	R	264	GLY	2.3
1	G	64	LEU	2.3
1	O	135	LYS	2.3
1	D	97	SER	2.3
1	K	64	LEU	2.3
1	D	191	ASP	2.3
1	P	63	PRO	2.3
1	P	169	SER	2.3
1	H	245	GLY	2.3
1	O	258	ALA	2.2
1	H	254	GLU	2.2
1	G	53	PRO	2.2
1	T	52	GLN	2.2
1	L	194	GLY	2.2
1	C	262	ARG	2.2
1	O	199	GLN	2.2
1	O	182	ILE	2.2
1	Q	273	ALA	2.2
1	T	192	GLU	2.2
1	B	262	ARG	2.2
1	O	133	ASN	2.2
1	B	189	GLY	2.2
1	I	261	LYS	2.2
1	L	261	LYS	2.2
1	T	135	LYS	2.2
1	D	192	GLU	2.2
1	E	48	ASN	2.2
1	K	53	PRO	2.2
1	L	50	HIS	2.2
1	M	46	HIS	2.2
1	O	53	PRO	2.1
1	S	124	SER	2.1
1	J	61	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	251	ILE	2.1
1	P	66	ALA	2.1
1	H	111	GLU	2.1
1	T	155	GLU	2.1
1	C	53	PRO	2.1
1	M	60	GLN	2.1
1	Q	2	GLN	2.1
1	L	133	ASN	2.1
1	B	191	ASP	2.1
1	E	111	GLU	2.1
1	J	262	ARG	2.1
1	Q	61	PRO	2.1
1	D	199	GLN	2.1
1	A	98	ASP	2.0
1	T	191	ASP	2.0
1	R	223	GLU	2.0
1	N	61	PRO	2.0
1	A	195	GLN	2.0
1	Q	274	LEU	2.0
1	O	50	HIS	2.0
1	A	182	ILE	2.0
1	K	56	ILE	2.0
1	P	216	GLY	2.0
1	O	187	VAL	2.0
1	H	98	ASP	2.0
1	D	59	SER	2.0
1	S	62	MET	2.0
1	J	58	LEU	2.0
1	K	268	LEU	2.0
1	Q	272	LEU	2.0
1	P	46	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PGH	L	300	10/10	0.87	0.14	50,52,53,54	0
3	PGH	I	300	10/10	0.90	0.13	50,52,53,54	0
3	PGH	K	300	10/10	0.91	0.11	50,52,53,54	0
3	PGH	O	300	10/10	0.91	0.15	50,52,53,54	0
3	PGH	M	300	10/10	0.92	0.14	50,52,53,54	0
3	PGH	P	300	10/10	0.92	0.13	50,52,53,54	0
3	PGH	N	300	10/10	0.93	0.10	50,52,53,54	0
3	PGH	S	300	10/10	0.93	0.11	50,52,53,54	0
3	PGH	J	300	10/10	0.94	0.12	50,52,53,54	0
3	PGH	E	300	10/10	0.94	0.11	50,52,53,54	0
3	PGH	G	300	10/10	0.94	0.10	50,52,53,54	0
3	PGH	C	300	10/10	0.94	0.12	50,52,53,54	0
3	PGH	A	300	10/10	0.95	0.10	50,52,53,54	0
3	PGH	Q	300	10/10	0.95	0.12	50,52,53,54	0
3	PGH	F	300	10/10	0.95	0.10	50,52,53,54	0
3	PGH	B	300	10/10	0.96	0.08	50,52,53,54	0
3	PGH	H	300	10/10	0.96	0.11	50,52,53,54	0
3	PGH	D	300	10/10	0.96	0.12	50,52,53,54	0
3	PGH	T	300	10/10	0.96	0.11	50,52,53,54	0
2	ZN	K	275	1/1	0.97	0.10	35,35,35,35	0
3	PGH	R	300	10/10	0.97	0.09	50,52,53,54	0
2	ZN	O	275	1/1	0.99	0.12	35,35,35,35	0
2	ZN	P	275	1/1	0.99	0.04	34,34,34,34	0
2	ZN	S	275	1/1	0.99	0.03	33,33,33,33	0
2	ZN	T	275	1/1	0.99	0.04	33,33,33,33	0
2	ZN	J	275	1/1	0.99	0.09	35,35,35,35	0
2	ZN	C	275	1/1	0.99	0.07	32,32,32,32	0
2	ZN	L	275	1/1	0.99	0.09	35,35,35,35	0
2	ZN	N	275	1/1	0.99	0.08	35,35,35,35	0
2	ZN	H	275	1/1	1.00	0.04	32,32,32,32	0
2	ZN	I	275	1/1	1.00	0.05	34,34,34,34	0
2	ZN	B	275	1/1	1.00	0.03	32,32,32,32	0
2	ZN	A	275	1/1	1.00	0.07	32,32,32,32	0
2	ZN	D	275	1/1	1.00	0.04	32,32,32,32	0
2	ZN	M	275	1/1	1.00	0.04	33,33,33,33	0
2	ZN	E	275	1/1	1.00	0.03	32,32,32,32	0
2	ZN	F	275	1/1	1.00	0.02	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	G	275	1/1	1.00	0.02	34,34,34,34	0
2	ZN	Q	275	1/1	1.00	0.05	32,32,32,32	0
2	ZN	R	275	1/1	1.00	0.04	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.