Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:45 PM GMT

PDB ID	:	1GT7
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

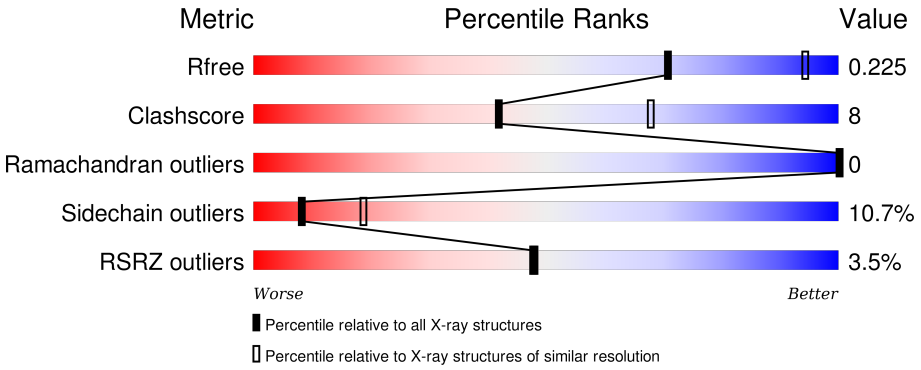
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	75% 19% 5%
1	B	274	76% 20%
1	C	274	75% 19% 6%
1	D	274	76% 18% 5%
1	E	274	76% 18% 5%

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Mol	Chain	Length	Quality of chain
1	F	274	79% 15% 6%
1	G	274	77% 18%
1	H	274	74% 19% 6%
1	I	274	4% 75% 20% 5%
1	J	274	8% 74% 20% 5%
1	K	274	12% 75% 19% 5%
1	L	274	8% 78% 16% 5%
1	M	274	3% 75% 19% 5%
1	N	274	5% 76% 17% 7%
1	O	274	14% 73% 22%
1	P	274	8% 74% 21%
1	Q	274	78% 16% 5%
1	R	274	77% 18% 5%
1	S	274	77% 18% 5%
1	T	274	75% 18% 6%

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	C	300	-	X	-	-
3	PGH	G	300	-	X	-	X
3	PGH	H	300	-	X	-	-
3	PGH	J	300	-	X	-	-
3	PGH	L	300	-	X	-	-
3	PGH	M	300	-	X	-	-
3	PGH	Q	300	-	X	-	-
3	PGH	T	300	-	X	-	-

2 Entry composition (i)

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	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	R	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	S	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			
1	T	274	Total	C	N	O	S	0	0	0
			2124	1358	361	394	11			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	1	Total	Zn	0	0
			1	1		
2	G	1	Total	Zn	0	0
			1	1		
2	J	1	Total	Zn	0	0
			1	1		
2	Q	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	K	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	I	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	T	1	Total	Zn	0	0
			1	1		
2	N	1	Total	Zn	0	0
			1	1		
2	O	1	Total	Zn	0	0
			1	1		

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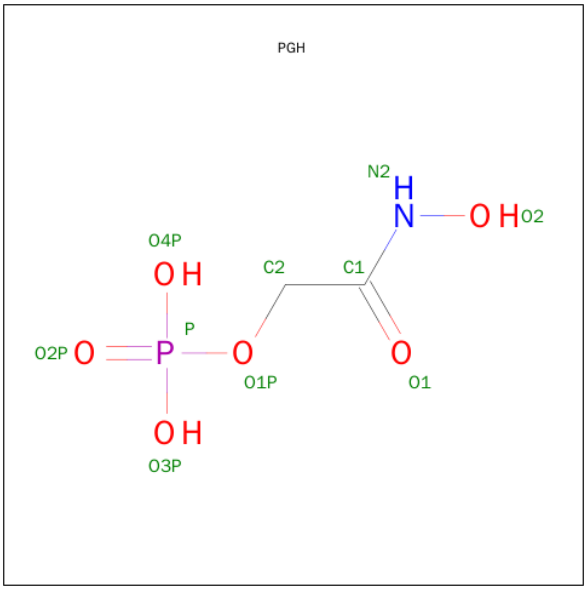
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	R	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0
2	S	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	M	1	Total Zn 1 1	0	0

- Molecule 3 is PHOSPHOGLYCOLOHYDROXAMIC ACID (three-letter code: PGH) (formula: $C_2H_6NO_6P$).



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

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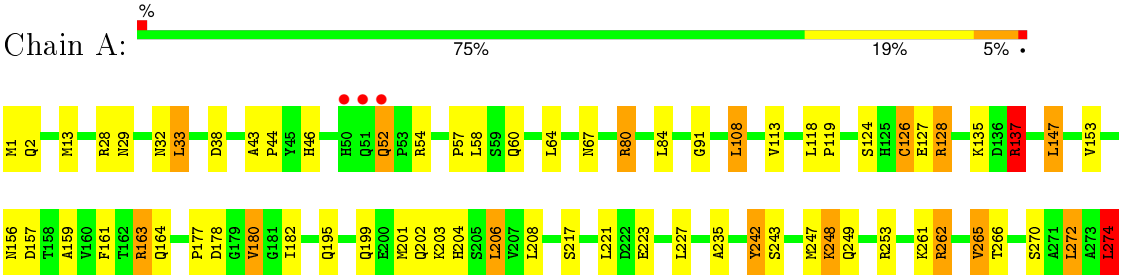
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	174	Total O 174 174	0	0
4	G	176	Total O 176 176	0	0
4	H	171	Total O 171 171	0	0
4	I	177	Total O 177 177	0	0
4	J	178	Total O 178 178	0	0
4	K	177	Total O 177 177	0	0
4	L	167	Total O 167 167	0	0
4	M	183	Total O 183 183	0	0
4	N	170	Total O 170 170	0	0
4	O	175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

3 Residue-property plots (i)

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

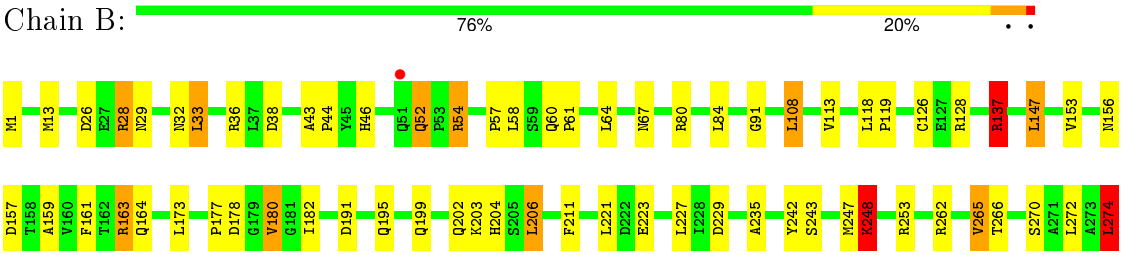
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain A:



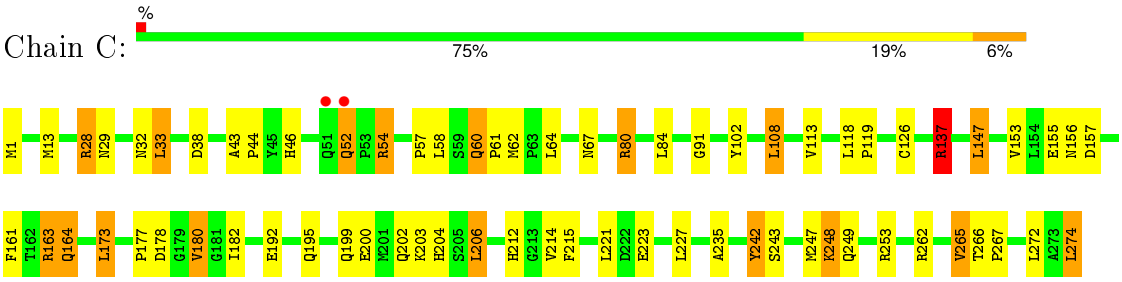
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain B:



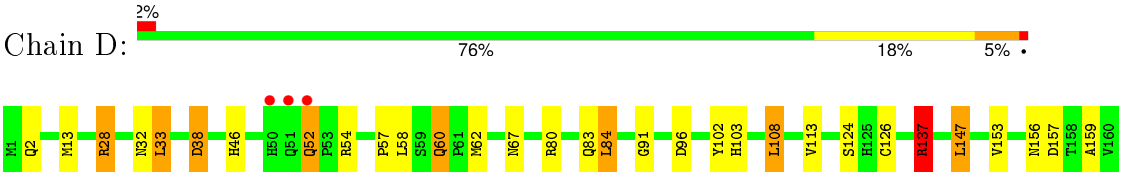
- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

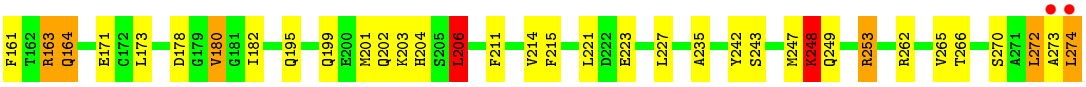
Chain C:



- Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

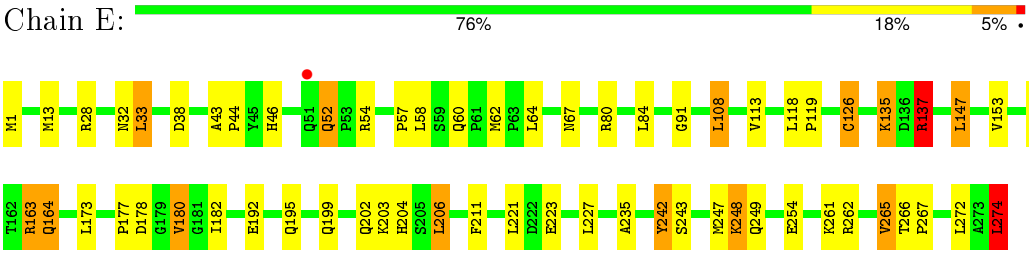
Chain D:





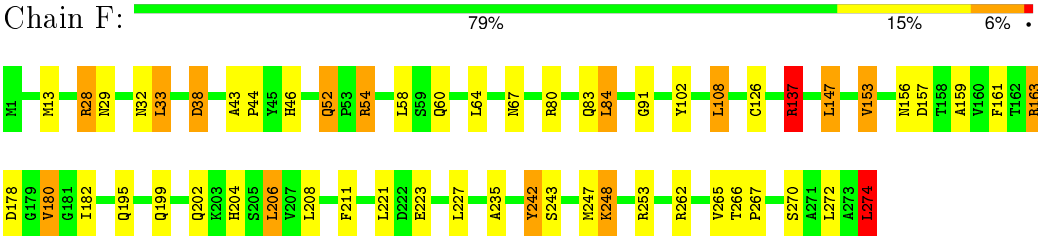
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain E:



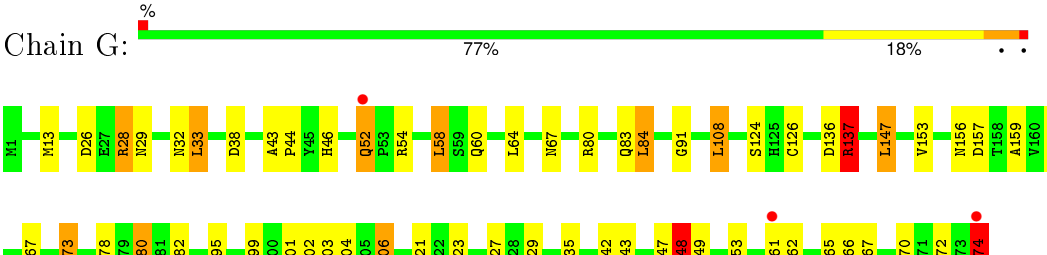
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain F:



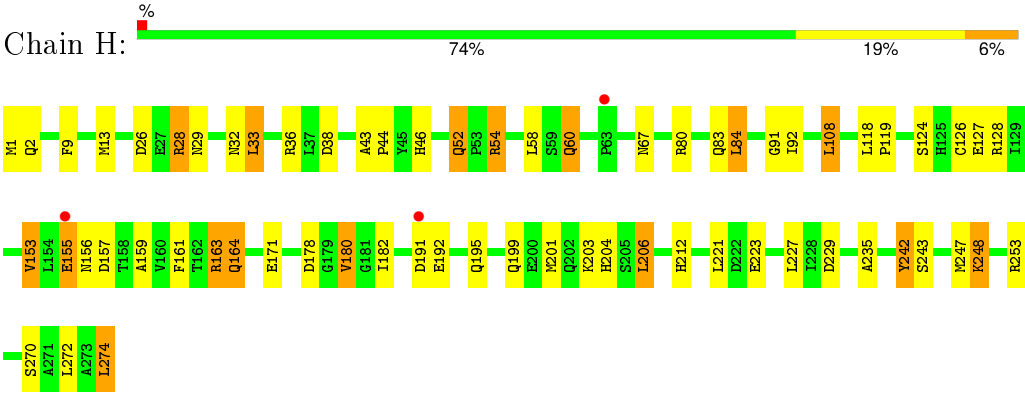
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain G:



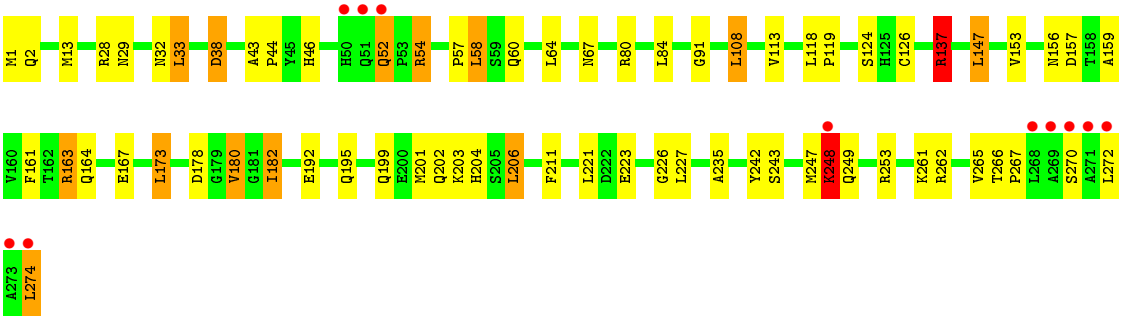
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain H:



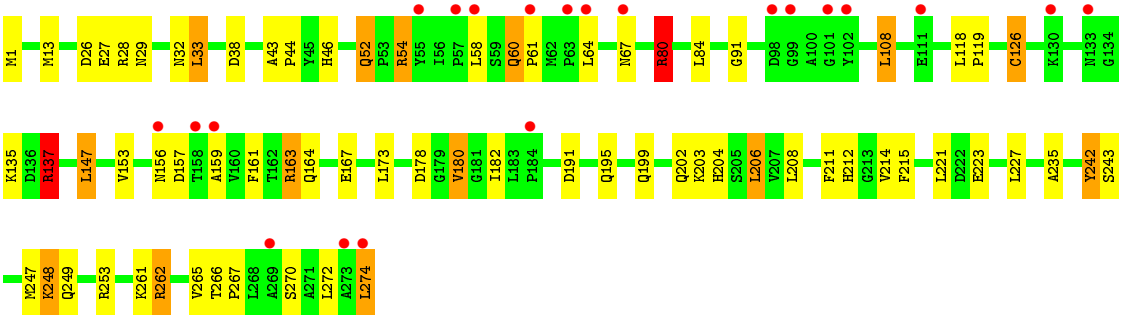
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain I:



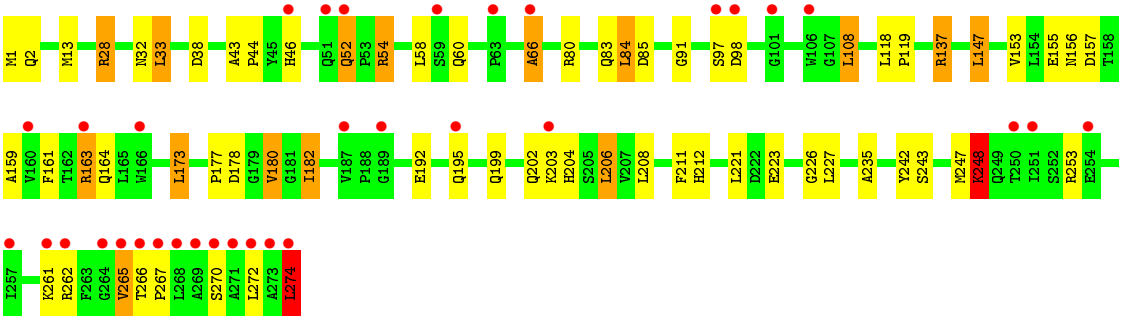
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain J:



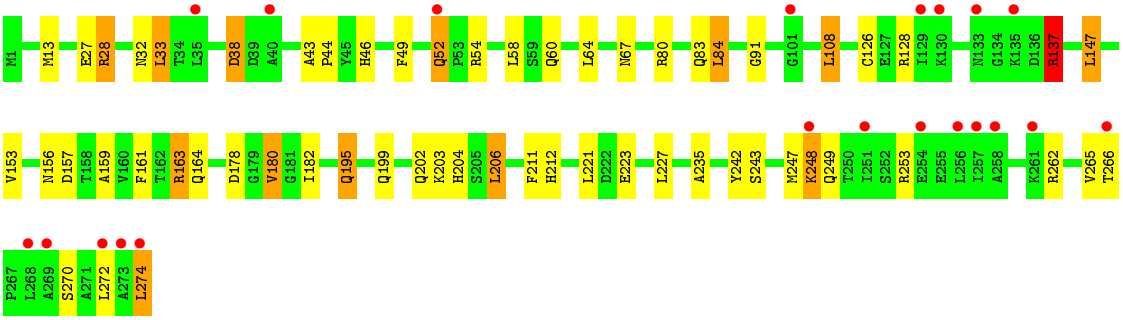
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain K:



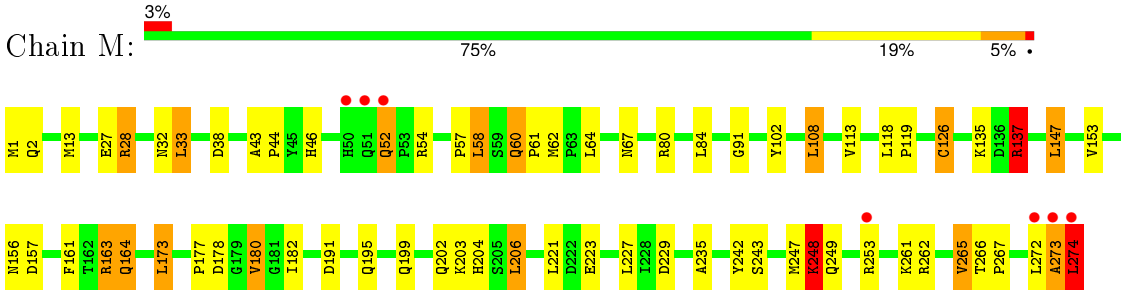
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain L:



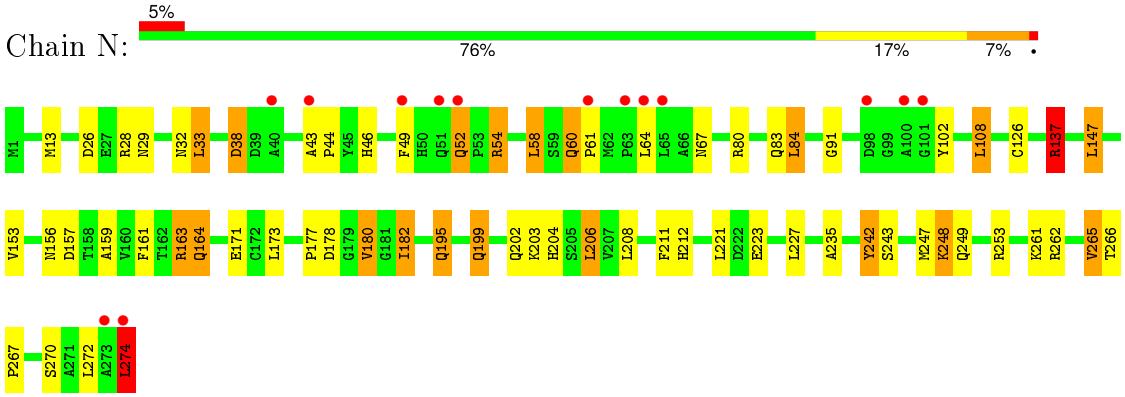
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain M:



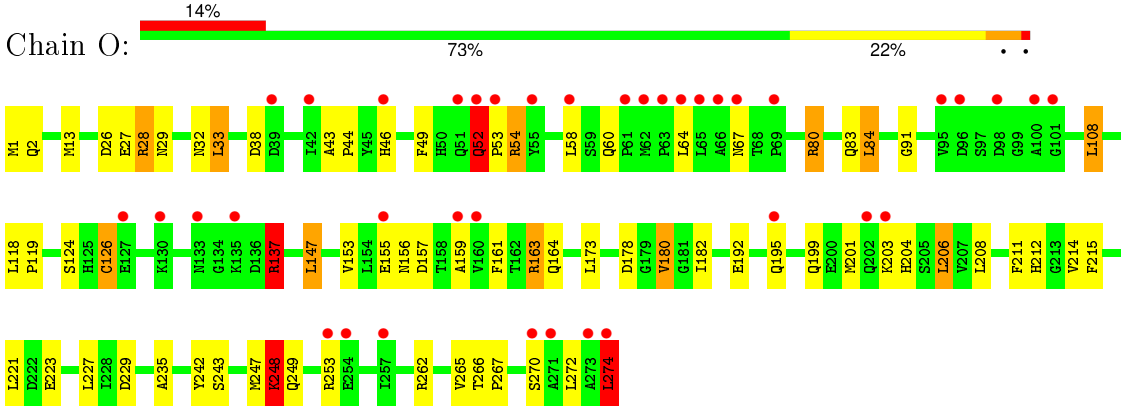
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain N:



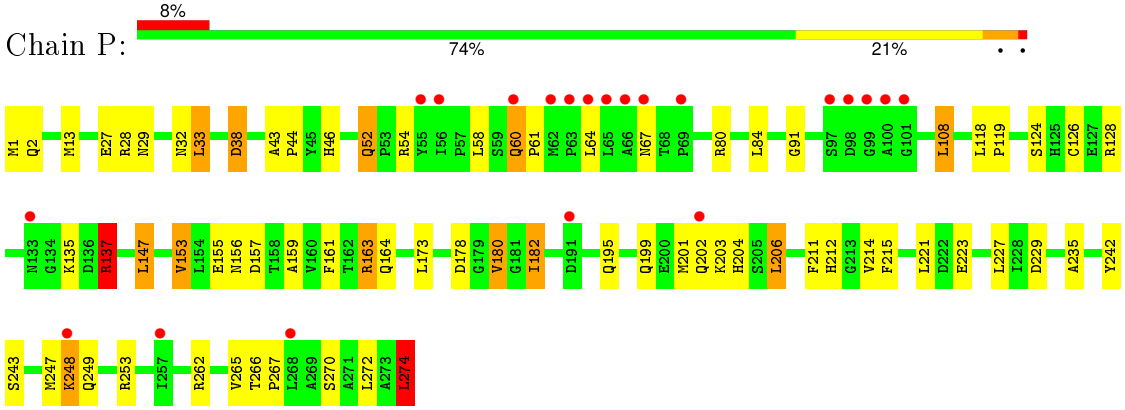
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain O:



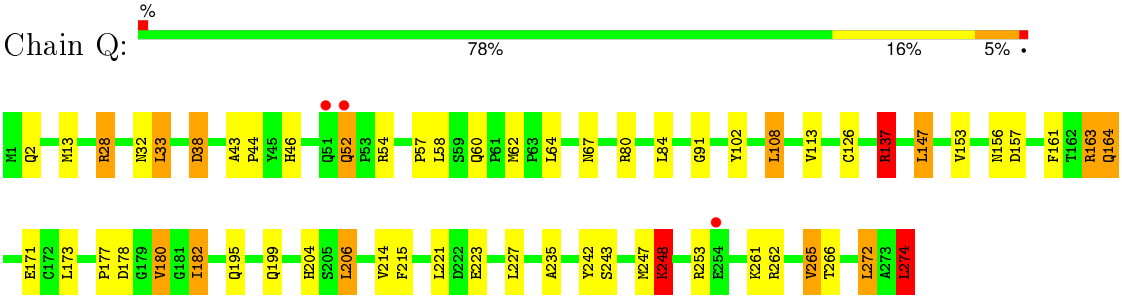
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain P:



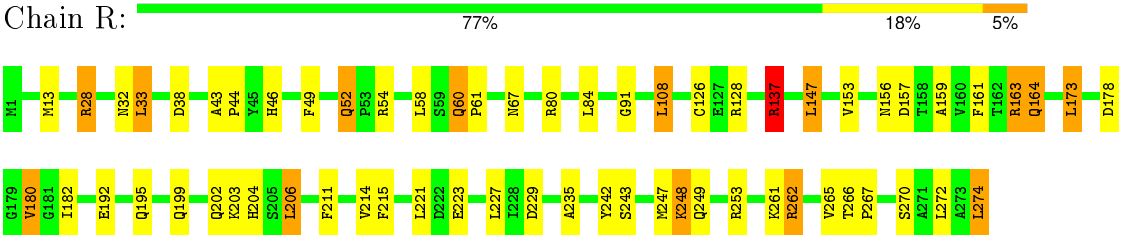
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain Q:



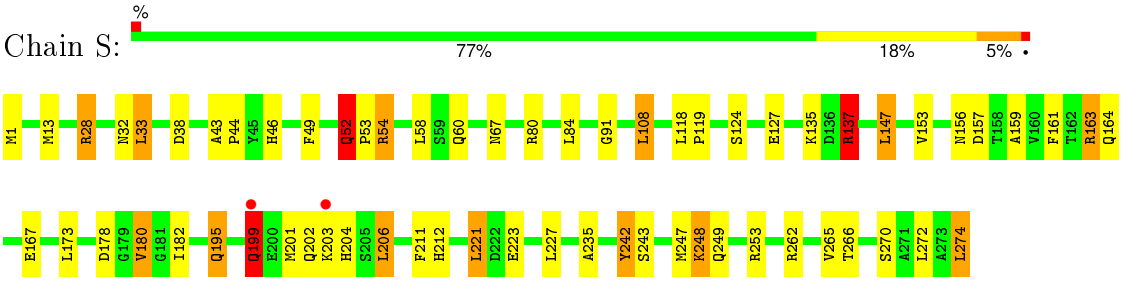
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain R:



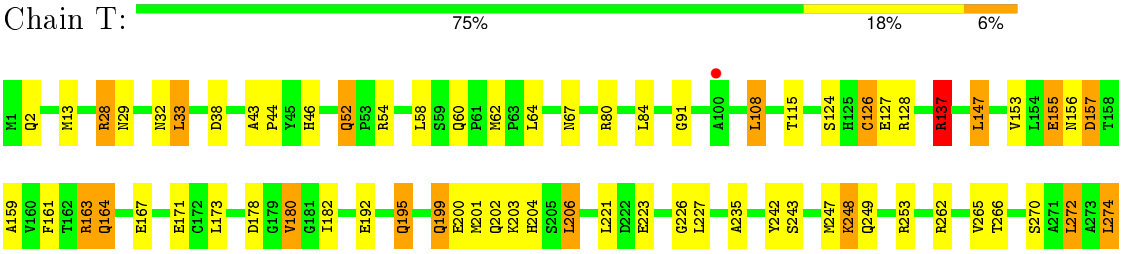
• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain S:



• Molecule 1: RHAMNULOSE-1-PHOSPHATE ALDOLASE

Chain T:



4 Data and refinement statistics (i)

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 44.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.3 (44.00-2.70) 90.3 (44.28-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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%)	DCC
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 , 34.8	EDS
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 207385 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.80	1/2178 (0.0%)	1.44	21/2966 (0.7%)
1	B	0.79	1/2178 (0.0%)	1.41	24/2966 (0.8%)
1	C	0.78	0/2178	1.47	27/2966 (0.9%)
1	D	0.81	1/2178 (0.0%)	1.47	24/2966 (0.8%)
1	E	0.77	1/2178 (0.0%)	1.37	21/2966 (0.7%)
1	F	0.76	1/2178 (0.0%)	1.40	24/2966 (0.8%)
1	G	0.76	1/2178 (0.0%)	1.40	21/2966 (0.7%)
1	H	0.82	2/2178 (0.1%)	1.46	30/2966 (1.0%)
1	I	0.81	0/2178	1.37	18/2966 (0.6%)
1	J	0.85	0/2178	1.40	21/2966 (0.7%)
1	K	0.98	1/2178 (0.0%)	1.41	20/2966 (0.7%)
1	L	0.93	0/2178	1.42	18/2966 (0.6%)
1	M	0.80	2/2178 (0.1%)	1.45	23/2966 (0.8%)
1	N	0.85	1/2178 (0.0%)	1.38	23/2966 (0.8%)
1	O	0.98	1/2178 (0.0%)	1.40	23/2966 (0.8%)
1	P	0.91	2/2178 (0.1%)	1.35	20/2966 (0.7%)
1	Q	0.81	1/2178 (0.0%)	1.43	24/2966 (0.8%)
1	R	0.78	0/2178	1.39	24/2966 (0.8%)
1	S	0.77	0/2178	1.39	23/2966 (0.8%)
1	T	0.78	0/2178	1.41	25/2966 (0.8%)
All	All	0.83	16/43560 (0.0%)	1.41	454/59320 (0.8%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	274	LEU	C-OXT	10.31	1.43	1.23
1	P	274	LEU	C-OXT	10.03	1.42	1.23
1	B	274	LEU	C-OXT	9.77	1.42	1.23
1	N	274	LEU	C-OXT	9.67	1.41	1.23
1	K	274	LEU	C-OXT	9.05	1.40	1.23
1	Q	274	LEU	C-OXT	7.29	1.37	1.23
1	H	155	GLU	CD-OE1	7.11	1.33	1.25
1	G	274	LEU	C-OXT	6.77	1.36	1.23
1	F	274	LEU	C-OXT	6.74	1.36	1.23
1	E	274	LEU	C-OXT	6.32	1.35	1.23
1	P	27	GLU	CD-OE1	5.88	1.32	1.25
1	H	155	GLU	CD-OE2	5.83	1.32	1.25
1	D	253	ARG	CZ-NH2	5.29	1.40	1.33
1	M	274	LEU	C-OXT	5.09	1.33	1.23
1	A	274	LEU	C-OXT	5.05	1.32	1.23
1	M	274	LEU	C-O	5.01	1.32	1.23

All (454) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	163	ARG	NE-CZ-NH1	20.91	130.76	120.30
1	C	163	ARG	NE-CZ-NH2	-19.36	110.62	120.30
1	D	163	ARG	NE-CZ-NH2	-18.05	111.27	120.30
1	Q	253	ARG	NE-CZ-NH1	17.83	129.22	120.30
1	M	163	ARG	NE-CZ-NH2	-16.75	111.92	120.30
1	J	163	ARG	NE-CZ-NH2	-15.29	112.65	120.30
1	O	163	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	A	262	ARG	NE-CZ-NH1	13.95	127.27	120.30
1	I	262	ARG	NE-CZ-NH1	13.85	127.23	120.30
1	C	163	ARG	NE-CZ-NH1	13.48	127.04	120.30
1	A	163	ARG	NE-CZ-NH2	-13.37	113.61	120.30
1	R	163	ARG	NE-CZ-NH2	-13.32	113.64	120.30
1	L	163	ARG	NE-CZ-NH2	-13.28	113.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	163	ARG	NE-CZ-NH2	-13.20	113.70	120.30
1	H	262	ARG	NE-CZ-NH1	13.13	126.86	120.30
1	L	262	ARG	NE-CZ-NH1	13.12	126.86	120.30
1	I	253	ARG	NE-CZ-NH1	13.02	126.81	120.30
1	B	163	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	D	163	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	C	253	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	G	163	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	N	253	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	J	262	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	N	163	ARG	NE-CZ-NH1	12.73	126.66	120.30
1	N	163	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	G	262	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	T	253	ARG	NE-CZ-NH1	12.47	126.54	120.30
1	T	163	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	F	163	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	F	253	ARG	NE-CZ-NH1	12.03	126.31	120.30
1	A	253	ARG	NE-CZ-NH1	11.99	126.30	120.30
1	H	157	ASP	CB-CG-OD1	11.94	129.05	118.30
1	I	163	ARG	NE-CZ-NH2	-11.76	114.42	120.30
1	R	253	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	L	163	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	F	163	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	D	262	ARG	NE-CZ-NH2	11.48	126.04	120.30
1	Q	163	ARG	NE-CZ-NH2	-11.48	114.56	120.30
1	C	262	ARG	NE-CZ-NH1	11.29	125.94	120.30
1	G	253	ARG	NE-CZ-NH1	11.20	125.90	120.30
1	Q	253	ARG	NE-CZ-NH2	-11.05	114.78	120.30
1	J	163	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	E	163	ARG	NE-CZ-NH2	-10.93	114.83	120.30
1	K	163	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	E	262	ARG	NE-CZ-NH2	10.76	125.68	120.30
1	L	253	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	D	262	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	P	262	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	F	262	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	T	262	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	G	28	ARG	NE-CZ-NH1	10.43	125.51	120.30
1	J	253	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	262	ARG	NH1-CZ-NH2	-10.33	108.03	119.40
1	C	28	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	B	223	GLU	OE1-CD-OE2	10.17	135.51	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	262	ARG	NH1-CZ-NH2	-10.07	108.33	119.40
1	A	223	GLU	OE1-CD-OE2	10.06	135.37	123.30
1	B	262	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	B	253	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	S	163	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	D	223	GLU	OE1-CD-OE2	9.87	135.15	123.30
1	S	253	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	M	262	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	R	262	ARG	NE-CZ-NH2	9.77	125.18	120.30
1	K	66	ALA	CB-CA-C	9.63	124.54	110.10
1	C	262	ARG	NH1-CZ-NH2	-9.53	108.92	119.40
1	H	262	ARG	NH1-CZ-NH2	-9.43	109.03	119.40
1	H	253	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	H	163	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	L	262	ARG	NH1-CZ-NH2	-9.31	109.16	119.40
1	O	223	GLU	OE1-CD-OE2	9.30	134.46	123.30
1	T	28	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	C	262	ARG	NE-CZ-NH2	9.21	124.90	120.30
1	S	223	GLU	OE1-CD-OE2	9.04	134.15	123.30
1	A	163	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	R	223	GLU	OE1-CD-OE2	8.90	133.98	123.30
1	M	262	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	K	253	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	S	163	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	L	223	GLU	OE1-CD-OE2	8.74	133.78	123.30
1	K	223	GLU	OE1-CD-OE2	8.58	133.60	123.30
1	A	262	ARG	NE-CZ-NH2	8.56	124.58	120.30
1	M	262	ARG	NH1-CZ-NH2	-8.54	110.01	119.40
1	S	262	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	H	223	GLU	OE1-CD-OE2	8.42	133.40	123.30
1	O	163	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	I	223	GLU	OE1-CD-OE2	8.37	133.34	123.30
1	O	262	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	F	262	ARG	NH1-CZ-NH2	-8.31	110.26	119.40
1	P	223	GLU	OE1-CD-OE2	8.31	133.27	123.30
1	P	163	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	P	262	ARG	NH1-CZ-NH2	-8.24	110.33	119.40
1	H	137	ARG	NE-CZ-NH2	8.22	124.41	120.30
1	M	223	GLU	OE1-CD-OE2	8.21	133.16	123.30
1	Q	262	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	P	163	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	C	223	GLU	OE1-CD-OE2	8.15	133.09	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	262	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	Q	223	GLU	OE1-CD-OE2	8.15	133.07	123.30
1	E	223	GLU	OE1-CD-OE2	8.13	133.06	123.30
1	T	223	GLU	OE1-CD-OE2	8.09	133.01	123.30
1	B	262	ARG	NH1-CZ-NH2	-8.09	110.50	119.40
1	L	137	ARG	CD-NE-CZ	8.06	134.89	123.60
1	S	157	ASP	CB-CG-OD1	8.05	125.55	118.30
1	C	28	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	G	137	ARG	CD-NE-CZ	8.01	134.81	123.60
1	D	157	ASP	CB-CG-OD1	7.99	125.49	118.30
1	O	253	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	G	262	ARG	NH1-CZ-NH2	-7.96	110.65	119.40
1	F	137	ARG	CD-NE-CZ	7.94	134.71	123.60
1	A	80	ARG	NE-CZ-NH1	-7.89	116.35	120.30
1	E	262	ARG	NH1-CZ-NH2	-7.89	110.72	119.40
1	I	262	ARG	NH1-CZ-NH2	-7.88	110.74	119.40
1	J	262	ARG	NH1-CZ-NH2	-7.87	110.75	119.40
1	G	223	GLU	OE1-CD-OE2	7.82	132.68	123.30
1	N	262	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	T	262	ARG	NH1-CZ-NH2	-7.80	110.82	119.40
1	H	191	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	K	262	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	262	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	R	128	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	Q	262	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	E	137	ARG	CD-NE-CZ	7.74	134.44	123.60
1	E	137	ARG	NE-CZ-NH2	7.73	124.17	120.30
1	G	28	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	F	262	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	E	38	ASP	CB-CA-C	-7.66	95.08	110.40
1	L	137	ARG	NE-CZ-NH2	7.65	124.13	120.30
1	Q	163	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	H	262	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	Q	137	ARG	CD-NE-CZ	7.58	134.22	123.60
1	R	262	ARG	NH1-CZ-NH2	-7.55	111.09	119.40
1	P	262	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	O	38	ASP	CB-CA-C	-7.51	95.38	110.40
1	G	38	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	J	38	ASP	CB-CA-C	-7.48	95.44	110.40
1	T	157	ASP	CB-CG-OD1	7.41	124.97	118.30
1	C	38	ASP	CB-CA-C	-7.39	95.61	110.40
1	C	137	ARG	CD-NE-CZ	7.39	133.95	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	28	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	N	137	ARG	CD-NE-CZ	7.39	133.94	123.60
1	M	38	ASP	CB-CA-C	-7.38	95.64	110.40
1	K	157	ASP	CB-CG-OD1	7.38	124.94	118.30
1	H	38	ASP	CB-CA-C	-7.37	95.66	110.40
1	E	163	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	P	52	GLN	CB-CG-CD	7.31	130.59	111.60
1	P	128	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	N	52	GLN	CB-CG-CD	7.29	130.55	111.60
1	Q	157	ASP	CB-CG-OD1	7.29	124.86	118.30
1	N	157	ASP	CB-CG-OD1	7.28	124.85	118.30
1	N	262	ARG	NH1-CZ-NH2	-7.28	111.40	119.40
1	L	38	ASP	CB-CA-C	-7.28	95.85	110.40
1	F	223	GLU	OE1-CD-OE2	7.25	132.00	123.30
1	T	192	GLU	OE1-CD-OE2	-7.25	114.61	123.30
1	F	28	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	G	38	ASP	CB-CA-C	-7.24	95.92	110.40
1	Q	262	ARG	NH1-CZ-NH2	-7.24	111.44	119.40
1	L	262	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	N	54	ARG	CD-NE-CZ	7.22	133.71	123.60
1	J	223	GLU	OE1-CD-OE2	7.22	131.96	123.30
1	R	229	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	137	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	R	223	GLU	CG-CD-OE2	-7.18	103.93	118.30
1	A	137	ARG	CD-NE-CZ	7.18	133.65	123.60
1	F	52	GLN	CB-CG-CD	7.16	130.22	111.60
1	A	223	GLU	CG-CD-OE2	-7.15	104.00	118.30
1	I	137	ARG	CD-NE-CZ	7.14	133.60	123.60
1	O	262	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	H	38	ASP	CB-CG-OD1	-7.11	111.90	118.30
1	G	163	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	S	199	GLN	N-CA-CB	-7.05	97.91	110.60
1	O	262	ARG	NH1-CZ-NH2	-7.03	111.66	119.40
1	T	38	ASP	CB-CA-C	-7.03	96.35	110.40
1	Q	38	ASP	CB-CA-C	-7.01	96.37	110.40
1	J	54	ARG	CD-NE-CZ	6.99	133.38	123.60
1	R	38	ASP	CB-CA-C	-6.98	96.43	110.40
1	E	249	GLN	N-CA-CB	6.98	123.17	110.60
1	O	249	GLN	N-CA-CB	6.95	123.11	110.60
1	B	38	ASP	CB-CA-C	-6.95	96.51	110.40
1	N	38	ASP	CB-CA-C	-6.94	96.52	110.40
1	O	157	ASP	CB-CG-OD1	6.93	124.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	137	ARG	CD-NE-CZ	6.91	133.28	123.60
1	T	163	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	J	137	ARG	CD-NE-CZ	6.91	133.27	123.60
1	A	38	ASP	CB-CA-C	-6.91	96.59	110.40
1	J	80	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	F	253	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	H	52	GLN	CB-CG-CD	6.84	129.38	111.60
1	N	223	GLU	OE1-CD-OE2	6.83	131.50	123.30
1	P	38	ASP	CB-CA-C	-6.82	96.75	110.40
1	S	54	ARG	CD-NE-CZ	6.81	133.14	123.60
1	S	262	ARG	NH1-CZ-NH2	-6.78	111.94	119.40
1	B	28	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	D	38	ASP	CB-CA-C	-6.76	96.89	110.40
1	L	157	ASP	CB-CG-OD1	6.76	124.38	118.30
1	S	38	ASP	CB-CA-C	-6.75	96.90	110.40
1	I	163	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	R	163	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	T	137	ARG	CD-NE-CZ	6.70	132.98	123.60
1	F	38	ASP	CB-CA-C	-6.68	97.03	110.40
1	R	54	ARG	CD-NE-CZ	6.63	132.89	123.60
1	I	38	ASP	CB-CA-C	-6.62	97.16	110.40
1	L	52	GLN	CB-CG-CD	6.62	128.80	111.60
1	R	137	ARG	CD-NE-CZ	6.61	132.86	123.60
1	B	52	GLN	CB-CG-CD	6.58	128.71	111.60
1	Q	52	GLN	CB-CG-CD	6.57	128.69	111.60
1	F	242	TYR	CB-CG-CD2	6.55	124.93	121.00
1	T	262	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	O	54	ARG	CD-NE-CZ	6.54	132.75	123.60
1	E	62	MET	CG-SD-CE	6.50	110.60	100.20
1	R	164	GLN	CA-CB-CG	6.49	127.67	113.40
1	C	137	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	K	38	ASP	CB-CA-C	-6.47	97.47	110.40
1	A	157	ASP	CB-CG-OD1	6.45	124.10	118.30
1	R	128	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	P	137	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	D	38	ASP	CB-CG-OD1	-6.44	112.50	118.30
1	C	249	GLN	N-CA-CB	6.44	122.19	110.60
1	R	52	GLN	CB-CG-CD	6.41	128.28	111.60
1	H	137	ARG	CD-NE-CZ	6.41	132.57	123.60
1	S	262	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	242	TYR	CB-CG-CD2	6.39	124.84	121.00
1	A	249	GLN	N-CA-CB	6.39	122.11	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	262	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	128	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	R	262	ARG	CD-NE-CZ	6.35	132.50	123.60
1	I	38	ASP	CB-CG-OD1	-6.35	112.58	118.30
1	I	157	ASP	CB-CG-OD1	6.35	124.02	118.30
1	F	38	ASP	CB-CG-OD1	-6.32	112.61	118.30
1	M	249	GLN	N-CA-CB	6.32	121.97	110.60
1	K	52	GLN	CB-CG-CD	6.31	128.02	111.60
1	M	248	LYS	CB-CA-C	6.30	123.01	110.40
1	S	52	GLN	CB-CG-CD	6.30	127.97	111.60
1	G	229	ASP	CB-CG-OD1	6.29	123.96	118.30
1	R	192	GLU	OE1-CD-OE2	-6.29	115.75	123.30
1	H	163	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	137	ARG	CD-NE-CZ	6.26	132.37	123.60
1	I	223	GLU	CG-CD-OE2	-6.26	105.78	118.30
1	F	28	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	K	262	ARG	NH1-CZ-NH2	-6.22	112.55	119.40
1	J	52	GLN	CB-CG-CD	6.20	127.73	111.60
1	O	229	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	223	GLU	CG-CD-OE2	-6.20	105.90	118.30
1	P	229	ASP	CB-CG-OD1	6.20	123.88	118.30
1	J	223	GLU	CG-CD-OE2	-6.19	105.93	118.30
1	O	137	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	52	GLN	CB-CG-CD	6.14	127.55	111.60
1	M	157	ASP	CB-CG-OD1	6.14	123.82	118.30
1	L	54	ARG	CD-NE-CZ	6.13	132.19	123.60
1	O	192	GLU	OE1-CD-OE2	-6.12	115.96	123.30
1	B	157	ASP	CB-CG-OD1	6.12	123.80	118.30
1	D	52	GLN	CB-CG-CD	6.11	127.50	111.60
1	E	262	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	T	223	GLU	CG-CD-OE2	-6.11	106.08	118.30
1	B	262	ARG	CD-NE-CZ	6.10	132.14	123.60
1	H	155	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	F	223	GLU	CG-CD-OE2	-6.09	106.13	118.30
1	M	223	GLU	CG-CD-OE2	-6.08	106.14	118.30
1	C	157	ASP	CB-CG-OD1	6.06	123.75	118.30
1	B	128	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	O	52	GLN	CB-CG-CD	6.04	127.29	111.60
1	B	223	GLU	CG-CD-OE2	-6.03	106.24	118.30
1	B	137	ARG	CD-NE-CZ	6.03	132.04	123.60
1	C	62	MET	CG-SD-CE	5.99	109.78	100.20
1	M	28	ARG	NE-CZ-NH2	-5.98	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	137	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	D	171	GLU	OE1-CD-OE2	-5.96	116.14	123.30
1	H	28	ARG	CD-NE-CZ	5.96	131.95	123.60
1	S	49	PHE	CB-CG-CD2	5.96	124.97	120.80
1	Q	248	LYS	CB-CA-C	5.96	122.31	110.40
1	E	223	GLU	CG-CD-OE2	-5.95	106.40	118.30
1	I	52	GLN	CB-CG-CD	5.95	127.07	111.60
1	J	249	GLN	N-CA-CB	5.94	121.29	110.60
1	H	26	ASP	CB-CG-OD2	5.94	123.64	118.30
1	K	262	ARG	NE-CZ-NH2	5.92	123.26	120.30
1	H	36	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	G	137	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	L	38	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	K	66	ALA	N-CA-CB	-5.89	101.86	110.10
1	J	137	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	G	52	GLN	CB-CG-CD	5.87	126.87	111.60
1	J	191	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	E	164	GLN	CA-CB-CG	5.86	126.29	113.40
1	N	54	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	C	155	GLU	OE1-CD-OE2	5.85	130.32	123.30
1	Q	223	GLU	CG-CD-OE2	-5.85	106.60	118.30
1	E	52	GLN	CB-CG-CD	5.84	126.80	111.60
1	N	38	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	O	223	GLU	CG-CD-OE2	-5.84	106.62	118.30
1	K	38	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	E	38	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	E	262	ARG	CD-NE-CZ	5.82	131.74	123.60
1	I	137	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	F	157	ASP	CB-CG-OD1	5.81	123.53	118.30
1	E	157	ASP	CB-CG-OD1	5.80	123.52	118.30
1	I	249	GLN	N-CA-CB	5.79	121.02	110.60
1	D	262	ARG	CD-NE-CZ	5.79	131.71	123.60
1	D	62	MET	CG-SD-CE	5.79	109.46	100.20
1	A	54	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	T	171	GLU	OE1-CD-OE2	-5.78	116.36	123.30
1	O	137	ARG	CD-NE-CZ	5.77	131.68	123.60
1	F	242	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	P	157	ASP	CB-CG-OD1	5.75	123.48	118.30
1	P	223	GLU	CG-CD-OE2	-5.75	106.80	118.30
1	Q	38	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	C	80	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	Q	171	GLU	OE1-CD-OE2	-5.73	116.42	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	28	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	M	38	ASP	CB-CG-OD1	-5.71	113.17	118.30
1	L	223	GLU	CG-CD-OE2	-5.70	106.90	118.30
1	D	248	LYS	O-C-N	-5.69	113.60	122.70
1	J	157	ASP	CB-CG-OD1	5.68	123.42	118.30
1	F	164	GLN	CA-CB-CG	5.68	125.89	113.40
1	R	38	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	K	262	ARG	CD-NE-CZ	5.64	131.50	123.60
1	G	54	ARG	CD-NE-CZ	5.64	131.49	123.60
1	D	249	GLN	N-CA-CB	5.62	120.71	110.60
1	O	26	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	128	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	R	157	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	S	137	ARG	CD-NE-CZ	5.61	131.45	123.60
1	C	52	GLN	CB-CG-CD	5.60	126.17	111.60
1	D	28	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	J	26	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	262	ARG	CD-NE-CZ	5.59	131.43	123.60
1	C	253	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	G	248	LYS	CB-CA-C	5.58	121.57	110.40
1	E	54	ARG	CD-NE-CZ	5.58	131.41	123.60
1	B	54	ARG	CD-NE-CZ	5.57	131.40	123.60
1	O	262	ARG	CD-NE-CZ	5.56	131.39	123.60
1	T	249	GLN	N-CA-CB	5.56	120.61	110.60
1	D	272	LEU	O-C-N	-5.55	113.81	122.70
1	S	199	GLN	CB-CG-CD	-5.55	97.16	111.60
1	P	153	VAL	N-CA-CB	-5.55	99.30	111.50
1	L	249	GLN	N-CA-CB	5.54	120.58	110.60
1	S	28	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	Q	272	LEU	CA-CB-CG	5.53	128.02	115.30
1	D	164	GLN	CA-CB-CG	5.51	125.51	113.40
1	H	192	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	M	191	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	T	52	GLN	CB-CG-CD	5.50	125.90	111.60
1	S	223	GLU	CG-CD-OE2	-5.50	107.31	118.30
1	E	126	CYS	CB-CA-C	5.49	121.38	110.40
1	L	28	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	G	223	GLU	CG-CD-OE2	-5.49	107.33	118.30
1	M	52	GLN	CB-CG-CD	5.47	125.83	111.60
1	R	249	GLN	N-CA-CB	5.47	120.45	110.60
1	F	54	ARG	CD-NE-CZ	5.47	131.26	123.60
1	G	157	ASP	CB-CG-OD2	-5.45	113.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	223	GLU	CG-CD-OE2	-5.45	107.40	118.30
1	H	137	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
1	Q	182	ILE	CB-CA-C	-5.43	100.73	111.60
1	K	155	GLU	OE1-CD-OE2	5.41	129.80	123.30
1	N	102	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	J	126	CYS	CB-CA-C	5.40	121.20	110.40
1	I	192	GLU	OE1-CD-OE2	-5.40	116.83	123.30
1	C	223	GLU	CG-CD-OE2	-5.39	107.53	118.30
1	K	54	ARG	CD-NE-CZ	5.37	131.11	123.60
1	Q	28	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	H	242	TYR	CB-CG-CD2	5.36	124.22	121.00
1	M	137	ARG	CD-NE-CZ	5.36	131.10	123.60
1	H	28	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	R	126	CYS	CB-CA-C	5.36	121.11	110.40
1	H	223	GLU	CG-CD-OE2	-5.35	107.59	118.30
1	T	62	MET	CG-SD-CE	5.35	108.76	100.20
1	G	26	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	26	ASP	CB-CG-OD2	5.34	123.10	118.30
1	L	253	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	36	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	B	38	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	T	137	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	102	TYR	CB-CG-CD2	5.33	124.20	121.00
1	C	54	ARG	CD-NE-CZ	5.33	131.06	123.60
1	N	164	GLN	CA-CB-CG	5.33	125.12	113.40
1	K	28	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	T	128	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	I	182	ILE	CB-CA-C	-5.31	100.98	111.60
1	G	249	GLN	N-CA-CB	5.31	120.15	110.60
1	C	192	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	I	54	ARG	CD-NE-CZ	5.30	131.02	123.60
1	N	182	ILE	CB-CA-C	-5.30	101.00	111.60
1	G	157	ASP	CB-CG-OD1	5.30	123.07	118.30
1	T	164	GLN	CA-CB-CG	5.30	125.06	113.40
1	F	102	TYR	CB-CG-CD2	5.29	124.17	121.00
1	P	249	GLN	N-CA-CB	5.29	120.12	110.60
1	C	164	GLN	CA-CB-CG	5.28	125.02	113.40
1	B	248	LYS	O-C-N	-5.28	114.26	122.70
1	J	80	ARG	NH1-CZ-NH2	5.28	125.20	119.40
1	T	200	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	M	273	ALA	N-CA-CB	5.26	117.47	110.10
1	T	28	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	242	TYR	CB-CG-CD2	5.26	124.16	121.00
1	H	229	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	P	155	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	K	223	GLU	CG-CD-OE2	-5.24	107.81	118.30
1	H	54	ARG	CD-NE-CZ	5.24	130.93	123.60
1	O	248	LYS	CB-CA-C	5.22	120.85	110.40
1	E	192	GLU	OE1-CD-OE2	-5.21	117.04	123.30
1	P	182	ILE	CB-CA-C	-5.21	101.17	111.60
1	D	102	TYR	CB-CG-CD2	5.21	124.13	121.00
1	S	221	LEU	O-C-N	-5.21	114.36	122.70
1	E	242	TYR	CB-CG-CD2	5.21	124.13	121.00
1	B	229	ASP	CB-CG-OD1	5.19	122.97	118.30
1	M	62	MET	CG-SD-CE	5.19	108.51	100.20
1	Q	102	TYR	CB-CG-CD2	5.19	124.11	121.00
1	N	26	ASP	CB-CG-OD2	5.18	122.97	118.30
1	Q	62	MET	CG-SD-CE	5.18	108.49	100.20
1	B	137	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	153	VAL	N-CA-CB	-5.18	100.11	111.50
1	K	182	ILE	CB-CA-C	-5.17	101.25	111.60
1	K	192	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	R	262	ARG	CB-CG-CD	5.17	125.05	111.60
1	P	253	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	R	28	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	Q	157	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	T	155	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	F	173	LEU	CA-CB-CG	5.16	127.16	115.30
1	N	242	TYR	CB-CG-CD2	5.16	124.09	121.00
1	T	126	CYS	CB-CA-C	5.15	120.71	110.40
1	M	229	ASP	CB-CG-OD1	5.15	122.94	118.30
1	N	171	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	M	164	GLN	CA-CB-CG	5.13	124.69	113.40
1	J	242	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	191	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	126	CYS	CB-CA-C	5.11	120.62	110.40
1	H	164	GLN	CA-CB-CG	5.11	124.65	113.40
1	C	200	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	J	27	GLU	OE1-CD-OE2	-5.10	117.18	123.30
1	Q	164	GLN	CA-CB-CG	5.10	124.63	113.40
1	S	157	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	S	242	TYR	CB-CG-CD2	5.09	124.05	121.00
1	S	249	GLN	N-CA-CB	5.09	119.76	110.60
1	S	242	TYR	CB-CG-CD1	-5.09	117.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	126	CYS	CB-CA-C	5.09	120.57	110.40
1	H	153	VAL	N-CA-CB	-5.09	100.31	111.50
1	M	248	LYS	O-C-N	-5.08	114.56	122.70
1	A	38	ASP	CB-CG-OD1	-5.08	113.72	118.30
1	M	126	CYS	CB-CA-C	5.08	120.56	110.40
1	F	262	ARG	CD-NE-CZ	5.08	130.71	123.60
1	N	157	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	248	LYS	CB-CA-C	5.07	120.53	110.40
1	I	248	LYS	CB-CA-C	5.07	120.53	110.40
1	D	206	LEU	CA-CB-CG	5.06	126.94	115.30
1	T	272	LEU	CA-CB-CG	5.06	126.94	115.30
1	O	80	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	H	171	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	N	249	GLN	N-CA-CB	5.04	119.68	110.60
1	D	96	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	272	LEU	CA-CB-CG	5.03	126.88	115.30
1	A	126	CYS	CB-CA-C	5.02	120.45	110.40
1	K	248	LYS	CB-CA-C	5.02	120.44	110.40
1	M	102	TYR	CB-CG-CD2	5.02	124.01	121.00
1	O	126	CYS	CB-CA-C	5.02	120.43	110.40
1	P	157	ASP	CB-CG-OD2	-5.01	113.79	118.30

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	39	0
1	B	2124	0	2097	32	0
1	C	2124	0	2097	33	0
1	D	2124	0	2097	36	2
1	E	2124	0	2097	33	1
1	F	2124	0	2097	30	0
1	G	2124	0	2097	35	0
1	H	2124	0	2097	38	1
1	I	2124	0	2097	38	0
1	J	2124	0	2097	37	0
1	K	2124	0	2097	41	8
1	L	2124	0	2097	33	2
1	M	2124	0	2097	40	2
1	N	2124	0	2097	40	0
1	O	2124	0	2097	39	0
1	P	2124	0	2097	37	0
1	Q	2124	0	2097	30	0
1	R	2124	0	2097	32	0
1	S	2124	0	2097	33	9
1	T	2124	0	2097	44	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
3	I	10	0	3	0	0
3	J	10	0	3	0	0
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	1	0
4	A	177	0	0	16	0
4	B	174	0	0	14	0
4	C	173	0	0	13	0
4	D	173	0	0	19	0
4	E	179	0	0	15	0
4	F	174	0	0	15	0
4	G	176	0	0	14	0
4	H	171	0	0	18	2
4	I	177	0	0	15	0
4	J	178	0	0	14	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	14	0
4	P	167	0	0	18	0
4	Q	176	0	0	14	0
4	R	172	0	0	15	1
4	S	171	0	0	15	0
4	T	170	0	0	25	0
All	All	46180	0	42000	707	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 8.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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	1.16
1:K:97:SER:HB3	4:K:2077:HOH:O	1.28	1.15
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:N:163:ARG:NH2	1:N:274:LEU:OXT	1.95	1.00
1:D:46:HIS:HB2	4:D:2054:HOH:O	1.61	1.00
1:T:157:ASP:OD1	4:T:2105:HOH:O	1.78	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: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:S:163:ARG:NH2	1:S:274:LEU:OXT	2.04	0.89
1:I:91:GLY:HA3	1:I:108:LEU:HD22	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:H:130:LYS:NZ	4:H:2101:HOH:O	2.10	0.83
1:T:157:ASP:OD2	4:T:2104:HOH:O	1.93	0.83
1:G:91:GLY:HA3	1:G:108:LEU:HD22	1.59	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:Q:46:HIS:HE1	4:Q:2065:HOH:O	1.64	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: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: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:D:243:SER:O	4:D:2152:HOH:O	1.99	0.79
1:E:91:GLY:HA3	1:E:108:LEU:HD22	1.63	0.78
1:O:247:MET:HE2	4:O:2159:HOH:O	1.83	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:D:46:HIS:HE1	4:D:2055:HOH:O	1.67	0.77
1:B:46:HIS:HB2	4:B:2062:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:T:243:SER:O	4:T:2150:HOH:O	2.03	0.75
1:P:243:SER:O	4:P:2147:HOH:O	2.03	0.75
1:A:147:LEU:HD13	1:A:235:ALA:HB2	1.68	0.75
1:S:46:HIS:HB2	4:S:2059:HOH:O	1.85	0.75
1:Q:164:GLN:NE2	4:Q:2120:HOH:O	2.18	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: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:L:178:ASP:O	1:L:204:HIS:HD2	1.70	0.74
1:B:113:VAL:HG11	1:I:57:PRO:HD3	1.69	0.74
1:S:91:GLY:HA3	1:S:108:LEU:HD22	1.68	0.74
1:O:147:LEU:HD13	1:O:235:ALA:HB2	1.70	0.74
1:I:147:LEU:HD13	1:I:235:ALA:HB2	1.68	0.74
1:E:178:ASP:O	1:E:204:HIS:HD2	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:S:28:ARG:HD2	4:S:2038:HOH:O	1.87	0.73
1:B:243:SER:O	4:B:2154:HOH:O	2.06	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:Q:247:MET:HE2	4:Q:2164:HOH:O	1.88	0.72
1:I:178:ASP:O	1:I:204:HIS:HD2	1.71	0.72
1:R:28:ARG:HD2	4:R:2037:HOH:O	1.90	0.72
1:N:147:LEU:HD13	1:N: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:K:147:LEU:HD13	1:K:235:ALA:HB2	1.70	0.72
1:H:60:GLN:OE1	4:H:2068:HOH:O	0.72	0.71
1:T:147:LEU:HD13	1:T:235:ALA:HB2	1.71	0.71
1:N:28:ARG:HD2	4:N:2036:HOH:O	1.90	0.71
1:O:243:SER:O	4:O:2155:HOH:O	2.07	0.71
1:J:46:HIS:HB2	4:J:2062:HOH:O	1.88	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:H:247:MET:HE2	4:H:2156:HOH:O	1.90	0.70
1:Q:178:ASP:O	1:Q:204:HIS:HD2	1.73	0.70
1:S:243:SER:O	4:S:2151:HOH:O	2.09	0.70
1:F:147:LEU:HD13	1:F:235:ALA:HB2	1.73	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: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:P:247:MET:HE2	4:P:2151:HOH:O	1.90	0.69
1:T:247:MET:HE2	4:T:2154:HOH:O	1.93	0.69
1:J:147:LEU:HD13	1:J:235:ALA:HB2	1.73	0.69
1:G:164:GLN:NE2	4:G:2116:HOH:O	2.24	0.69
1:C:243:SER:O	4:C:2153:HOH:O	2.10	0.69
1:B:28:ARG:HD2	4:B:2041:HOH:O	1.90	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:G:243:SER:O	4:G:2156:HOH:O	2.13	0.67
1:M:243:SER:O	4:M:2163:HOH:O	2.12	0.67
1:A:243:SER:O	4:A:2158:HOH:O	2.13	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:L:247:MET:HE2	4:L:2151:HOH:O	1.93	0.67
1:T:164:GLN:NE2	4:T:2109:HOH:O	2.28	0.66
1:D:67:ASN:HB2	4:D:2071:HOH:O	1.95	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:I:247:MET:HE2	4:I:2161:HOH:O	1.95	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: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: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: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:K:46:HIS:HE1	4:K:2063:HOH:O	1.81	0.63
1:E:67:ASN:HB2	4:E:2080:HOH:O	1.99	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:A:247:MET:HE2	4:A:2161:HOH:O	1.99	0.62
1:T:28:ARG:HD2	4:T:2036:HOH:O	1.99	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:S:67:ASN:HB2	4:S:2074:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:247:MET:HE2	4:K:2161:HOH:O	2.01	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:M:164:GLN:NE2	4:M:2124:HOH:O	2.35	0.60
1:G:247:MET:HE2	4:G:2160:HOH:O	2.02	0.60
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:G:67:ASN:HB2	4:G:2076:HOH:O	2.01	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:B:247:MET:HE2	4:B:2158: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:J:247:MET:HE2	4:J:2162:HOH:O	2.03	0.57
1:D:247:MET:HE2	4:D:2156:HOH:O	2.05	0.57
1:Q:248:LYS:CE	4:Q:2166:HOH:O	2.52	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:T:156:ASN:HB3	4:T:2118:HOH:O	2.04	0.57
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:K:248:LYS:NZ	4:K:2163:HOH:O	2.22	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:S:137:ARG:HD3	4:S:2052:HOH:O	2.04	0.56
1:D:248:LYS:NZ	4:D:2157:HOH:O	2.19	0.56
1:O:180:VAL:HB	1:O:206:LEU:HB3	1.87	0.56
1:E:164:GLN:NE2	4:E:2122:HOH:O	2.37	0.56
1:K:164:GLN:NE2	4:K:2119:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASN:HB2	4:B:2076:HOH:O	2.05	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: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:E:247:MET:HE2	4:E:2164:HOH:O	2.06	0.55
1:L:13:MET:SD	1:L:33:LEU:HD13	2.45	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:N:202:GLN:HG2	4:N:2099:HOH:O	2.06	0.55
1:M:137:ARG:HD3	4:M:2058:HOH:O	2.06	0.55
1:O:206:LEU:HD22	1:O:227:LEU:HD11	1.88	0.55
1:K:206:LEU:HD22	1:K:227:LEU:HD11	1.89	0.55
1:M:67:ASN:HB2	4:M:2082:HOH:O	2.07	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:D:253:ARG:NH2	4:D:2161:HOH:O	2.38	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:N:247:MET:HE2	4:N:2154:HOH:O	2.06	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:S:247:MET:HE2	4:S:2155:HOH:O	2.08	0.54
1:I:164:GLN:NE2	1:I:242:TYR:OH	2.40	0.54
1:Q:13:MET:SD	1:Q:33:LEU:HD13	2.47	0.54
1:O:13:MET:SD	1:O:33:LEU:HD13	2.47	0.54
1:L:206:LEU:HD22	1:L:227:LEU:HD11	1.89	0.54
1:J:137:ARG:HD3	4:J:2052:HOH:O	2.07	0.54
1:A:64:LEU:HD23	1:A:126:CYS:SG	2.47	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:C:247:MET:HE2	4:C:2157:HOH:O	2.09	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:J:13:MET:SD	1:J:33:LEU:HD13	2.48	0.53
1:G:180:VAL:HB	1:G:206:LEU:HB3	1.90	0.53
1:F:248:LYS:NZ	4:F:2159:HOH:O	2.23	0.53
1:S:164:GLN:NE2	1:S:242:TYR:OH	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:248:LYS:NZ	4:G:2162:HOH:O	2.20	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:L:248:LYS:NZ	4:L:2152:HOH:O	2.24	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:M:247:MET:HE2	4:M:2167:HOH:O	2.09	0.52
1:O:156:ASN:HB3	4:O:2124:HOH:O	2.08	0.52
1:A:206:LEU:HD22	1:A:227:LEU:HD11	1.92	0.52
1:K:247:MET:HE2	4:K:2119:HOH:O	2.09	0.52
1:N:180:VAL:HB	1:N:206:LEU:HB3	1.90	0.52
1:C:137:ARG:HD3	4:C:2052:HOH:O	2.08	0.52
1:S:13:MET:SD	1:S:33:LEU:HD13	2.49	0.52
1:R:180:VAL:HB	1:R:206:LEU:HB3	1.90	0.52
1:L:164:GLN:NE2	1:L:242:TYR:OH	2.42	0.52
1:D:180:VAL:HB	1:D:206:LEU:HB3	1.91	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: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:D:13:MET:SD	1:D:33:LEU:HD13	2.49	0.52
1:F:164:GLN:NE2	4:F:2115:HOH:O	2.43	0.52
1:L:137:ARG:HD3	4:L:2047:HOH:O	2.08	0.52
1:A:137:ARG:HD3	4:A:2057:HOH:O	2.10	0.52
1:A:13:MET:SD	1:A:33:LEU:HD13	2.49	0.52
1:I:43:ALA:HB3	1:I:44:PRO:HD3	1.92	0.52
1:E:180:VAL:HB	1:E:206:LEU:HB3	1.92	0.52
1:C:156:ASN:HB3	4:C:2123:HOH:O	2.10	0.52
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: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:A:164:GLN:NE2	1:A:242:TYR:OH	2.40	0.51
1:F:54:ARG:HD3	4:F:2069:HOH:O	2.10	0.51
1:K:248:LYS:CE	4:K:2163:HOH:O	2.56	0.51
1:D:54:ARG:HD3	4:D:2066:HOH:O	2.08	0.51
1:C:180:VAL:HB	1:C:206:LEU:HB3	1.91	0.51
1:P:206:LEU:HD22	1:P:227:LEU:HD11	1.91	0.51
1:F:164:GLN:NE2	1:F:242:TYR:OH	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:202:GLN:HG2	4:L:2095: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: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:F:248:LYS:CE	4:F:2159:HOH:O	2.59	0.51
1:B:164:GLN:NE2	1:B:242:TYR:OH	2.42	0.51
1:P:13:MET:SD	1:P:33:LEU:HD13	2.51	0.51
1:C:164:GLN:NE2	4:C:2115:HOH:O	2.44	0.51
1:C:164:GLN:NE2	1:C:242:TYR:OH	2.40	0.51
1:M:13:MET:SD	1:M:33:LEU:HD13	2.51	0.51
1:B:180:VAL:HB	1:B:206:LEU:HB3	1.92	0.51
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:H:137:ARG:HD3	4:H:2048:HOH:O	2.11	0.50
1:B:248:LYS:CE	4:B:2160:HOH:O	2.58	0.50
1:P:248:LYS:NZ	4:P:2152:HOH:O	2.27	0.50
1:P:159:ALA:HB2	1:P:270:SER:HB2	1.93	0.50
1:D:164:GLN:NE2	1:D:242:TYR:OH	2.41	0.50
1:B:43:ALA:HB3	1:B:44:PRO:HD3	1.93	0.50
1:M:164:GLN:NE2	1:M:242:TYR:OH	2.38	0.50
1:G:248:LYS:CE	4:G:2162:HOH:O	2.59	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:Q:180:VAL:HB	1:Q:206:LEU:HB3	1.94	0.50
1:J:180:VAL:HB	1:J: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:T:206:LEU:HD22	1:T:227:LEU:HD11	1.94	0.49
1:L:43:ALA:HB3	1:L:44:PRO:HD3	1.92	0.49
1:J:164:GLN:NE2	1:J:242:TYR:OH	2.43	0.49
1:B:164:GLN:NE2	4:B:2115:HOH:O	2.45	0.49
1:R:247:MET:HE2	4:R:2156:HOH:O	2.12	0.49
1:E:64:LEU:HD23	1:E:126:CYS:SG	2.52	0.49
1:H:206:LEU:HD22	1:H:227:LEU:HD11	1.93	0.49
1:E:248:LYS:CE	4:E:2165:HOH:O	2.59	0.49
1:M:180:VAL:HB	1:M:206:LEU:HB3	1.94	0.49
1:A:1:MET:HB3	4:A:2069:HOH:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:180:VAL:HB	1:F:206:LEU:HB3	1.94	0.49
1:A:180:VAL:HB	1:A:206:LEU:HB3	1.95	0.49
1:P:248:LYS:CE	4:P:2152:HOH:O	2.59	0.49
1:P:43:ALA:HB3	1:P:44:PRO:HD3	1.95	0.49
1:L:147:LEU:HD13	1:L:235:ALA:CB	2.41	0.48
1:L:247:MET:HE2	4:L:2107:HOH:O	2.11	0.48
1:T:13:MET:SD	1:T:33:LEU:HD13	2.53	0.48
1:G:13:MET:SD	1:G:33:LEU:HD13	2.53	0.48
1:T:248:LYS:CE	4:T:2155:HOH:O	2.59	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:O:173:LEU:HD21	1:O:267:PRO:HB3	1.96	0.48
1:N:247:MET:HE2	4:N:2110:HOH:O	2.13	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:K:43:ALA:HB3	1:K:44:PRO:HD3	1.95	0.48
1:Q:2:GLN:HG3	4:Q:2003:HOH:O	2.13	0.48
1:M:54:ARG:HD3	4:M:2076:HOH:O	2.12	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
1:F:247:MET:HE2	4:F:2158:HOH:O	2.13	0.48
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:T:202:GLN:HG2	4:T:2094:HOH:O	2.12	0.48
1:I:54:ARG:HD3	4:I:2072:HOH:O	2.14	0.48
1:M:156:ASN:HB3	4:M:2118:HOH:O	2.13	0.48
1:C:113:VAL:HG11	1:M:57:PRO:HD3	1.94	0.48
1:A:57:PRO:HD3	1:E:113:VAL:HG11	1.96	0.48
1:Q:156:ASN:HB3	4:Q:2129:HOH:O	2.13	0.48
1:B:1:MET:HB3	4:B:2065:HOH:O	2.13	0.48
1:T:115:THR:OG1	3:T:300:PGH:O2P	2.27	0.48
1:O:248:LYS:NZ	4:O:2160:HOH:O	2.16	0.48
1:Q:43:ALA:HB3	1:Q:44:PRO:HD3	1.95	0.47
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:R:206:LEU:HD22	1:R:227:LEU:HD11	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:202:GLN:HG2	4:I:2107:HOH:O	2.14	0.47
1:T:2:GLN:HG3	4:T:2002:HOH:O	2.14	0.47
1:F:137:ARG:HD3	4:F:2050:HOH:O	2.14	0.47
1:T:46:HIS:CE1	4:T:2056:HOH:O	2.57	0.47
1:M:1:MET:HB3	4:M:2070:HOH:O	2.14	0.47
1:L:203:LYS:HE3	1:L:203:LYS:HB2	1.66	0.47
1:S:180:VAL:HB	1:S:206:LEU:HB3	1.95	0.47
1:T:137:ARG:HD3	4:T:2047:HOH:O	2.13	0.47
1:J:203:LYS:HE3	1:J:203:LYS:HB2	1.71	0.47
1:P:46:HIS:CE1	4:P:2050:HOH:O	2.57	0.47
1:E:164:GLN:NE2	1:E:242:TYR:OH	2.42	0.47
1:A:156:ASN:HB3	4:A:2127:HOH:O	2.15	0.47
1:P:202:GLN:HG2	4:P:2095:HOH:O	2.14	0.47
1:N:43:ALA:HB3	1:N:44:PRO:HD3	1.97	0.47
1:J:1:MET:HB3	4:J:2065:HOH:O	2.15	0.47
1:C:64:LEU:HD23	1:C:126:CYS:SG	2.55	0.47
1:A:202:GLN:HG2	4:A:2106:HOH:O	2.15	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:G:136:ASP:OD1	4:G:2106:HOH:O	2.20	0.47
1:C:1:MET:HB3	4:C:2063:HOH:O	2.15	0.47
1:R:164:GLN:NE2	1:R:242:TYR:OH	2.42	0.47
1:I:206:LEU:HD22	1:I:227:LEU:HD11	1.96	0.47
1:A:203:LYS:HE3	1:A:203:LYS:HB2	1.61	0.47
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:B:64:LEU:HD23	1:B:126:CYS:SG	2.56	0.46
1:B:57:PRO:HD3	1:I:113:VAL:HG11	1.97	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:J:80:ARG:O	1:J:80:ARG:HD3	2.15	0.46
1:C:54:ARG:HD3	4:C:2071:HOH:O	2.13	0.46
1:B:118:LEU:N	1:B:119:PRO:CD	2.78	0.46
1:R:159:ALA:HB2	1:R:270:SER:HB2	1.98	0.46
1:G:159:ALA:HB2	1:G:270:SER:HB2	1.97	0.46
1:L:83:GLN:HG3	1:L:84:LEU:HD13	1.98	0.46
1:H:1:MET:HB3	4:H:2058:HOH:O	2.15	0.46
1:K:159:ALA:HB2	1:K:270:SER:HB2	1.98	0.46
1:T:159:ALA:HB2	1:T:270:SER:HB2	1.96	0.46
1:H:203:LYS:HB2	1:H:203:LYS:HE3	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:164:GLN:NE2	4:N:2110:HOH:O	2.49	0.46
1:G:137:ARG:HD3	4:G:2053:HOH:O	2.14	0.46
1:P:2:GLN:HG3	4:P:2002:HOH:O	2.15	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:T:248:LYS:NZ	4:T:2155:HOH:O	2.22	0.46
1:J:54:ARG:HD3	4:J:2070:HOH:O	2.16	0.46
1:F:64:LEU:HD23	1:F:126:CYS:SG	2.56	0.46
1:K:83:GLN:HG3	1:K:84:LEU:HD13	1.98	0.46
1:T:124:SER:HB3	1:T:201:MET:HG3	1.98	0.46
1:O:124:SER:HB3	1:O:201:MET:HG3	1.97	0.45
1:G:124:SER:HB3	1:G:201:MET:HG3	1.98	0.45
1:M:248:LYS:NZ	4:M:2170:HOH:O	2.29	0.45
4:Q:2165:HOH:O	1:T:155:GLU:HG3	2.16	0.45
1:N:173:LEU:HD21	1:N:267:PRO:HB3	1.98	0.45
1:O:203:LYS:HB2	1:O:203:LYS:HE3	1.66	0.45
1:I:203:LYS:HB2	1:I:203:LYS:HE3	1.68	0.45
1:I:64:LEU:HD23	1:I:126:CYS:SG	2.56	0.45
1:M:202:GLN:HG2	4:M:2111:HOH:O	2.16	0.45
1:A:118:LEU:N	1:A:119:PRO:CD	2.80	0.45
1:S:124:SER:HB3	1:S:201:MET:HG3	1.98	0.45
1:M:58:LEU:HD12	1:M:58:LEU:HA	1.79	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:D:206:LEU:HD22	1:D:227:LEU:HD11	1.98	0.45
1:J:164:GLN:NE2	4:J:2117:HOH:O	2.49	0.45
1:E:1:MET:HA	4:E:2002:HOH:O	2.16	0.45
1:D:57:PRO:HD3	1:Q:113:VAL:HG11	1.97	0.45
1:I:261:LYS:HB3	1:I:261:LYS:HE2	1.80	0.45
1:B:206:LEU:HD22	1:B:227:LEU:HD11	1.99	0.45
1:M:173:LEU:HD21	1:M:267:PRO:HB3	1.98	0.45
1:H:43:ALA:HB3	1:H:44:PRO:HD3	1.97	0.45
1:O:2:GLN:HG3	4:O:2002:HOH:O	2.16	0.45
1:I:159:ALA:HB2	1:I:270:SER:HB2	1.98	0.45
1:N:248:LYS:NZ	4:N:2155:HOH:O	2.10	0.45
1:A:43:ALA:HB3	1:A:44:PRO:HD3	1.97	0.45
1:J:173:LEU:HD21	1:J:267:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LYS:HE3	1:B:203:LYS:HB2	1.66	0.45
1:Q:261:LYS:HE2	1:Q:261:LYS:HB3	1.86	0.45
1:P:203:LYS:HB2	1:P:203:LYS:HE3	1.65	0.45
1:F:247:MET:HE2	4:F:2115:HOH:O	2.17	0.45
1:G:64:LEU:HD23	1:G:126:CYS:SG	2.56	0.45
1:M:247:MET:HE2	4:M:2124:HOH:O	2.17	0.44
1:M:2:GLN:HG3	4:M:2003:HOH:O	2.17	0.44
1:K:173:LEU:HD21	1:K:267:PRO:HB3	1.99	0.44
1:H:124:SER:HB3	1:H:201:MET:HG3	1.98	0.44
1:C:43:ALA:HB3	1:C:44:PRO:HD3	2.00	0.44
4:E:2166:HOH:O	1:H:155:GLU:HG3	2.16	0.44
1:E:261:LYS:HE2	1:E:261:LYS:HB3	1.91	0.44
1:G:178:ASP:O	1:G:204:HIS:CD2	2.55	0.44
1:J:28:ARG:HG3	1:K:226:GLY:HA3	1.99	0.44
1:N:178:ASP:O	1:N:204:HIS:CD2	2.62	0.44
1:A:164:GLN:NE2	4:A:2118:HOH:O	2.49	0.44
1:O:64:LEU:HD23	1:O:126:CYS:SG	2.58	0.44
1:K:54:ARG:HD3	4:K:2073:HOH:O	2.17	0.44
1:P:214:VAL:HG22	1:P:215:PHE:N	2.32	0.44
1:I:248:LYS:CE	4:I:2163:HOH:O	2.64	0.44
1:J:156:ASN:HB3	4:J:2125:HOH:O	2.16	0.44
1:M:203:LYS:HB2	1:M:203:LYS:HE3	1.64	0.44
1:J:43:ALA:HB3	1:J:44:PRO:HD3	1.98	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: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:S:43:ALA:HB3	1:S:44:PRO:HD3	1.99	0.44
1:C:248:LYS:CE	4:C:2159:HOH:O	2.66	0.44
1:K:261:LYS:HB3	1:K:261:LYS:HE2	1.84	0.44
1:P:178:ASP:O	1:P:204:HIS:CD2	2.60	0.44
1:M:248:LYS:HD2	4:M:2170:HOH:O	2.17	0.44
1:I:124:SER:HB3	1:I:201:MET:HG3	1.99	0.44
1:B:137:ARG:HD3	4:B:2053:HOH:O	2.18	0.44
1:A:113:VAL:HG11	1:E:57:PRO:HD3	2.00	0.44
1:H:28:ARG:HB3	1:H:29:ASN:H	1.58	0.44
1:P:248:LYS:HD2	4:P:2152:HOH:O	2.18	0.44
1:H:83:GLN:HG3	1:H:84:LEU:HD13	1.99	0.44
1:P:173:LEU:HD21	1:P:267:PRO:HB3	2.00	0.44
1:I:1:MET:HA	4:I:2002:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:28:ARG:HG3	1:T:226:GLY:HA3	1.99	0.43
1:A:262:ARG:HH11	1:A:262:ARG:HG3	1.83	0.43
1:L:64:LEU:HD23	1:L:126:CYS:SG	2.58	0.43
1:R:202:GLN:HG2	4:R:2099:HOH:O	2.18	0.43
1:B:159:ALA:HB2	1:B:270:SER:HB2	2.01	0.43
1:B:54:ARG:HD3	4:B:2071:HOH:O	2.17	0.43
1:P:164:GLN:NE2	4:P:2106:HOH:O	2.49	0.43
1:A:248:LYS:HD2	4:A:2163:HOH:O	2.17	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:D:124:SER:HB3	1:D:201:MET:HG3	2.00	0.43
1:L:27:GLU:HG2	1:L:27:GLU:O	2.17	0.43
1:E:173:LEU:HD21	1:E:267:PRO:HB3	2.00	0.43
1:M:248:LYS:CE	4:M:2170:HOH:O	2.65	0.43
1:J:214:VAL:HG22	1:J:215:PHE:N	2.33	0.43
1:I:58:LEU:HA	1:I:58:LEU:HD12	1.85	0.43
1:M:261:LYS:HB3	1:M:261:LYS:HE2	1.92	0.43
1:K:212:HIS:C	1:K:212:HIS:CD2	2.92	0.43
1:H:247:MET:HE2	4:H:2115:HOH:O	2.18	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:R:49:PHE:CD1	1:R:49:PHE:N	2.86	0.43
1:D:178:ASP:O	1:D:204:HIS:CD2	2.61	0.43
1:D:60:GLN:HB2	1:R:262:ARG:HD2	1.99	0.43
1:G:203:LYS:HE3	1:G:203:LYS:HB2	1.75	0.43
1:N:58:LEU:HA	1:N:58:LEU:HD12	1.83	0.43
1:O:147:LEU:HG	1:O:208:LEU:HD21	2.01	0.43
1:B:202:GLN:HG2	4:B:2103:HOH:O	2.18	0.43
1:M:1:MET:HA	4:M:2002:HOH:O	2.19	0.43
1:P:124:SER:HB3	1:P:201:MET:HG3	2.00	0.43
1:I:173:LEU:HD21	1:I:267:PRO:HB3	2.00	0.43
1:O:49:PHE:CD1	1:O:49:PHE:N	2.87	0.43
1:S:163:ARG:HD2	1:S:167:GLU:OE2	2.19	0.42
1:H:147:LEU:HD13	1:H:235:ALA:CB	2.47	0.42
1:F:147:LEU:HG	1:F:208:LEU:HD21	2.01	0.42
1:A:28:ARG:HB3	1:A:29:ASN:H	1.58	0.42
1:T:247:MET:HE2	4:T:2109:HOH:O	2.18	0.42
1:F:83:GLN:HG3	1:F:84:LEU:HD13	2.00	0.42
1:E:203:LYS:HE3	1:E:203:LYS:HB2	1.74	0.42
1:L:212:HIS:CD2	1:L:212:HIS:C	2.92	0.42
1:F:46:HIS:CE1	4:F:2058:HOH:O	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:HIS:CE1	4:A:2065:HOH:O	2.62	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:F:173:LEU:HD21	1:F:267:PRO:HB3	2.01	0.42
1:D:137:ARG:HD3	4:D:2047:HOH:O	2.18	0.42
1:J:212:HIS:CD2	1:J:212:HIS:C	2.90	0.42
1:A:147:LEU:HG	1:A:208:LEU:HD21	2.01	0.42
1:N:147:LEU:HG	1:N:208:LEU:HD21	2.01	0.42
1:Q:54:ARG:HD3	4:Q:2075:HOH:O	2.19	0.42
1:N:203:LYS:HB2	1:N:203:LYS:HE3	1.80	0.42
1:R:261:LYS:HB3	1:R:261:LYS:HE2	1.90	0.42
1:G:163:ARG:HD2	1:G:167:GLU:OE2	2.18	0.42
1:A:147:LEU:HD13	1:A:235:ALA:CB	2.44	0.42
1:L:178:ASP:O	1:L:204:HIS:CD2	2.61	0.42
1:I:248:LYS:NZ	4:I:2163:HOH:O	2.33	0.42
1:I:118:LEU:N	1:I:119:PRO:CD	2.82	0.42
1:R:173:LEU:HD21	1:R:267:PRO:HB3	2.01	0.42
1:E:157:ASP:O	1:E:158:THR:C	2.57	0.42
1:P:212:HIS:CD2	1:P:212:HIS:C	2.90	0.42
1:J:261:LYS:HE2	1:J:261:LYS:HB3	1.91	0.42
1:E:247:MET:HE2	4:E:2122:HOH:O	2.19	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
1:S:118:LEU:N	1:S:119:PRO:CD	2.82	0.42
1:M:118:LEU:N	1:M:119:PRO:CD	2.83	0.42
1:G:58:LEU:HD12	1:G:58:LEU:HA	1.83	0.42
1:R:247:MET:HE2	4:R:2110:HOH:O	2.18	0.42
1:I:137:ARG:HD3	4:I:2053:HOH:O	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:M:27:GLU:HG2	1:M:27:GLU:O	2.20	0.42
1:O:27:GLU:O	1:O:28:ARG:C	2.57	0.42
1:G:247:MET:HE2	4:G:2116:HOH:O	2.19	0.42
1:T:28:ARG:HB3	1:T:29:ASN:H	1.66	0.42
1:I:28:ARG:HB3	1:I:29:ASN:H	1.53	0.42
1:O:83:GLN:HG3	1:O:84:LEU:HD13	2.02	0.42
1:L:49:PHE:N	1:L:49:PHE:CD1	2.87	0.42
1:Q:177:PRO:HB3	1:Q:265:VAL:HG13	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:9:PHE:HE1	1:H:92:ILE:HD11	1.85	0.42
1:F:159:ALA:HB2	1:F:270:SER:HB2	2.02	0.42
1:P:28:ARG:HB3	1:P:29:ASN:H	1.64	0.41
1:A:159:ALA:HB2	1:A:270:SER:HB2	2.02	0.41
1:S:52:GLN:CD	1:S:52:GLN:H	2.23	0.41
1:G:83:GLN:HG3	1:G:84:LEU:HD13	2.02	0.41
1:G:261:LYS:HB3	1:G:261:LYS:HE2	1.89	0.41
1:K:177:PRO:HB3	1:K:265:VAL:HG13	2.01	0.41
1:F:28:ARG:HB3	1:F:29:ASN:H	1.60	0.41
1:C:28:ARG:HB3	1:C:29:ASN:H	1.55	0.41
1:Q:43:ALA:N	1:Q:44:PRO:CD	2.82	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:O:212:HIS:CD2	1:O:212:HIS:C	2.93	0.41
1:H:163:ARG:NH2	1:H:274:LEU:C	2.68	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:K:118:LEU:N	1:K:119:PRO:CD	2.84	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:N:64:LEU:HD23	1:N:126:CYS:SG	2.60	0.41
1:M:274:LEU:HA	1:M:274:LEU:HD12	1.87	0.41
1:K:147:LEU:HG	1:K:208:LEU:HD21	2.02	0.41
1:D:203:LYS:HB2	1:D:203:LYS:HE3	1.72	0.41
1:D:248:LYS:HD2	4:D:2157:HOH:O	2.21	0.41
1:D:214:VAL:HG22	1:D:215:PHE:N	2.36	0.41
1:M:64:LEU:HD23	1:M:126:CYS:SG	2.59	0.41
1:C:60:GLN:HA	1:C:61:PRO:HD3	1.94	0.41
1:J:60:GLN:HA	1:J:61:PRO:HD3	1.96	0.41
1:A:124:SER:HB3	1:A:201:MET:HG3	2.03	0.41
1:R:203:LYS:HE3	1:R:203:LYS:HB2	1.67	0.41
1:N:49:PHE:N	1:N:49:PHE:CD1	2.88	0.41
1:T:163:ARG:HD2	1:T:167:GLU:OE2	2.20	0.41
1:Q:248:LYS:NZ	4:Q:2166:HOH:O	2.23	0.41
1:O:1:MET:HG3	1:O:2:GLN:O	2.21	0.41
1:I:1:MET:HB3	4:I:2066:HOH:O	2.20	0.41
1:P:118:LEU:N	1:P:119:PRO:CD	2.82	0.41
1:M:177:PRO:HB3	1:M:265:VAL:HG13	2.02	0.41
1:N:177:PRO:HB3	1:N:265:VAL:HG13	2.02	0.41
1:B:177:PRO:HB3	1:B:265:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:43:ALA:HB3	1:O:44:PRO:HD3	2.01	0.41
1:R:214:VAL:HG22	1:R:215:PHE:N	2.36	0.41
1:C:177:PRO:HB3	1:C:265:VAL:HG13	2.02	0.41
1:A:261:LYS:HE2	1:A:261:LYS:HB3	1.87	0.41
1:N:60:GLN:HA	1:N:61:PRO:HD3	1.97	0.41
1:J:163:ARG:HD2	1:J:167:GLU:OE2	2.20	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:Q:214:VAL:HG22	1:Q:215:PHE:N	2.36	0.41
1:O:52:GLN:O	1:O:53:PRO:C	2.59	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:H:159:ALA:HB2	1:H:270:SER:HB2	2.02	0.41
1:D:159:ALA:HB2	1:D:270:SER:HB2	2.03	0.41
1:N:212:HIS:C	1:N:212:HIS:CD2	2.94	0.41
1:E:118:LEU:N	1:E:119:PRO:CD	2.84	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:M:163:ARG:NH2	1:M:274:LEU:C	2.74	0.41
1:D:2:GLN:HG3	4:D:2003:HOH:O	2.20	0.41
1:B:61:PRO:HD2	1:J:262:ARG:O	2.21	0.41
1:P:60:GLN:HA	1:P:61:PRO:HD3	1.96	0.40
1:H:54:ARG:HD3	4:H:2066:HOH:O	2.21	0.40
1:L:128:ARG:HD2	1:L:128:ARG:HA	1.90	0.40
1:L:159:ALA:HB2	1:L:270:SER:HB2	2.03	0.40
1:B:28:ARG:HB3	1:B:29:ASN:H	1.65	0.40
1:G:28:ARG:HB3	1:G:29:ASN:H	1.59	0.40
1:E:135:LYS:NZ	1:E:135:LYS:HB3	2.36	0.40
1:J:147:LEU:HG	1:J:208:LEU:HD21	2.03	0.40
1:S:52:GLN:O	1:S:53:PRO:C	2.60	0.40
1:O:214:VAL:HG22	1:O:215:PHE:N	2.36	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:O:54:ARG:HD3	4:O:2068:HOH:O	2.20	0.40
1:N:261:LYS:HB3	1:N:261:LYS:HE2	1.91	0.40
1:I:163:ARG:HD2	1:I:167:GLU:OE2	2.21	0.40
1:T:248:LYS:HD2	4:T:2155:HOH:O	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:C:212:HIS:CD2	1:C:212:HIS:C	2.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:212:HIS:CD2	1:S:212:HIS:C	2.94	0.40
1:T:157:ASP:HB2	4:T:2104:HOH:O	2.04	0.40
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:J:248:LYS:CE	4:J:2163:HOH:O	2.69	0.40
1:A:2:GLN:HG3	4:A:2004:HOH:O	2.21	0.40
1:M:60:GLN:HA	1:M:61:PRO:HD3	1.95	0.40
1:H:212:HIS:C	1:H:212:HIS:CD2	2.95	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:L:195:GLN:CD	1:L:195:GLN:CD[5_555]	2.18	0.02
1:K:66:ALA:N	1:S:199:GLN:NE2[1_655]	2.18	0.02
1:S:199:GLN:CG	4:K:2078:HOH:O[1_455]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	272/274 (99%)	264 (97%)	8 (3%)	0	100	100
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%)	204 (90%)	24 (10%)	8	19
1	B	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	C	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	D	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	E	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	F	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	G	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	H	228/228 (100%)	205 (90%)	23 (10%)	9	21
1	I	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	J	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	K	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	L	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	M	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	N	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	O	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	P	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	Q	228/228 (100%)	204 (90%)	24 (10%)	8	19
1	R	228/228 (100%)	203 (89%)	25 (11%)	8	18
1	S	228/228 (100%)	202 (89%)	26 (11%)	7	16
1	T	228/228 (100%)	204 (90%)	24 (10%)	8	19
All	All	4560/4560 (100%)	4070 (89%)	490 (11%)	8	19

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	LEU
1	A	52	GLN
1	A	58	LEU
1	A	60	GLN
1	A	80	ARG
1	A	84	LEU
1	A	108	LEU
1	A	135	LYS
1	A	137	ARG
1	A	147	LEU

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Mol	Chain	Res	Type
1	A	153	VAL
1	A	161	PHE
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	248	LYS
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	60	GLN
1	B	80	ARG
1	B	84	LEU
1	B	108	LEU
1	B	137	ARG
1	B	147	LEU
1	B	153	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	211	PHE
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

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Mol	Chain	Res	Type
1	C	60	GLN
1	C	80	ARG
1	C	84	LEU
1	C	108	LEU
1	C	137	ARG
1	C	147	LEU
1	C	153	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	248	LYS
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	80	ARG
1	D	84	LEU
1	D	108	LEU
1	D	137	ARG
1	D	147	LEU
1	D	153	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	211	PHE
1	D	221	LEU
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	60	GLN
1	E	80	ARG
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	161	PHE
1	E	180	VAL
1	E	182	ILE
1	E	195	GLN
1	E	199	GLN
1	E	206	LEU
1	E	211	PHE
1	E	221	LEU
1	E	248	LYS
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	60	GLN
1	F	80	ARG
1	F	84	LEU
1	F	108	LEU
1	F	137	ARG
1	F	147	LEU
1	F	153	VAL
1	F	161	PHE
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	211	PHE
1	F	221	LEU
1	F	248	LYS
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	60	GLN
1	G	80	ARG
1	G	84	LEU
1	G	108	LEU
1	G	137	ARG
1	G	147	LEU
1	G	153	VAL
1	G	161	PHE
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	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	80	ARG
1	H	84	LEU
1	H	108	LEU

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Mol	Chain	Res	Type
1	H	137	ARG
1	H	147	LEU
1	H	153	VAL
1	H	161	PHE
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	248	LYS
1	H	265	VAL
1	H	266	THR
1	H	272	LEU
1	H	274	LEU
1	I	32	ASN
1	I	33	LEU
1	I	52	GLN
1	I	58	LEU
1	I	60	GLN
1	I	80	ARG
1	I	84	LEU
1	I	108	LEU
1	I	137	ARG
1	I	147	LEU
1	I	153	VAL
1	I	161	PHE
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	211	PHE
1	I	221	LEU
1	I	248	LYS
1	I	265	VAL
1	I	266	THR
1	I	272	LEU
1	I	274	LEU
1	J	32	ASN
1	J	33	LEU

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Mol	Chain	Res	Type
1	J	52	GLN
1	J	58	LEU
1	J	60	GLN
1	J	80	ARG
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	161	PHE
1	J	180	VAL
1	J	182	ILE
1	J	195	GLN
1	J	199	GLN
1	J	206	LEU
1	J	211	PHE
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	60	GLN
1	K	80	ARG
1	K	84	LEU
1	K	108	LEU
1	K	137	ARG
1	K	147	LEU
1	K	153	VAL
1	K	161	PHE
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	211	PHE

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Mol	Chain	Res	Type
1	K	221	LEU
1	K	248	LYS
1	K	265	VAL
1	K	266	THR
1	K	272	LEU
1	K	274	LEU
1	L	32	ASN
1	L	33	LEU
1	L	52	GLN
1	L	58	LEU
1	L	60	GLN
1	L	80	ARG
1	L	84	LEU
1	L	108	LEU
1	L	137	ARG
1	L	147	LEU
1	L	153	VAL
1	L	161	PHE
1	L	180	VAL
1	L	182	ILE
1	L	195	GLN
1	L	199	GLN
1	L	206	LEU
1	L	211	PHE
1	L	221	LEU
1	L	248	LYS
1	L	265	VAL
1	L	266	THR
1	L	272	LEU
1	L	274	LEU
1	M	32	ASN
1	M	33	LEU
1	M	52	GLN
1	M	58	LEU
1	M	60	GLN
1	M	80	ARG
1	M	84	LEU
1	M	108	LEU
1	M	135	LYS
1	M	137	ARG
1	M	147	LEU
1	M	153	VAL

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Mol	Chain	Res	Type
1	M	161	PHE
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	60	GLN
1	N	80	ARG
1	N	84	LEU
1	N	108	LEU
1	N	137	ARG
1	N	147	LEU
1	N	153	VAL
1	N	161	PHE
1	N	180	VAL
1	N	182	ILE
1	N	195	GLN
1	N	199	GLN
1	N	206	LEU
1	N	211	PHE
1	N	221	LEU
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

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Mol	Chain	Res	Type
1	O	80	ARG
1	O	84	LEU
1	O	108	LEU
1	O	137	ARG
1	O	147	LEU
1	O	153	VAL
1	O	161	PHE
1	O	180	VAL
1	O	182	ILE
1	O	195	GLN
1	O	199	GLN
1	O	206	LEU
1	O	211	PHE
1	O	221	LEU
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	60	GLN
1	P	80	ARG
1	P	84	LEU
1	P	108	LEU
1	P	135	LYS
1	P	137	ARG
1	P	147	LEU
1	P	153	VAL
1	P	161	PHE
1	P	180	VAL
1	P	182	ILE
1	P	195	GLN
1	P	199	GLN
1	P	206	LEU
1	P	211	PHE
1	P	221	LEU
1	P	248	LYS
1	P	265	VAL
1	P	266	THR

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Mol	Chain	Res	Type
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	60	GLN
1	Q	80	ARG
1	Q	84	LEU
1	Q	108	LEU
1	Q	137	ARG
1	Q	147	LEU
1	Q	153	VAL
1	Q	161	PHE
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	248	LYS
1	Q	265	VAL
1	Q	266	THR
1	Q	272	LEU
1	Q	274	LEU
1	R	32	ASN
1	R	33	LEU
1	R	52	GLN
1	R	58	LEU
1	R	60	GLN
1	R	80	ARG
1	R	84	LEU
1	R	108	LEU
1	R	137	ARG
1	R	147	LEU
1	R	153	VAL
1	R	161	PHE
1	R	173	LEU
1	R	180	VAL
1	R	182	ILE
1	R	195	GLN

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Mol	Chain	Res	Type
1	R	199	GLN
1	R	206	LEU
1	R	211	PHE
1	R	221	LEU
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	60	GLN
1	S	80	ARG
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	161	PHE
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	211	PHE
1	S	221	LEU
1	S	248	LYS
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	60	GLN
1	T	80	ARG
1	T	84	LEU

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Mol	Chain	Res	Type
1	T	108	LEU
1	T	137	ARG
1	T	147	LEU
1	T	153	VAL
1	T	161	PHE
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	248	LYS
1	T	265	VAL
1	T	266	THR
1	T	272	LEU
1	T	274	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	164	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	60	GLN
1	D	156	ASN
1	D	164	GLN
1	D	195	GLN
1	D	204	HIS
1	E	156	ASN
1	E	164	GLN
1	E	204	HIS

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Mol	Chain	Res	Type
1	F	156	ASN
1	F	164	GLN
1	F	204	HIS
1	G	156	ASN
1	G	164	GLN
1	G	204	HIS
1	H	156	ASN
1	H	164	GLN
1	H	204	HIS
1	I	156	ASN
1	I	164	GLN
1	I	204	HIS
1	J	156	ASN
1	J	164	GLN
1	J	204	HIS
1	K	156	ASN
1	K	164	GLN
1	K	204	HIS
1	L	60	GLN
1	L	156	ASN
1	L	164	GLN
1	L	195	GLN
1	L	204	HIS
1	M	156	ASN
1	M	164	GLN
1	M	204	HIS
1	N	83	GLN
1	N	156	ASN
1	N	164	GLN
1	N	204	HIS
1	O	60	GLN
1	O	83	GLN
1	O	156	ASN
1	O	164	GLN
1	O	195	GLN
1	O	204	HIS
1	P	156	ASN
1	P	164	GLN
1	P	204	HIS
1	Q	156	ASN
1	Q	164	GLN
1	Q	204	HIS

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Mol	Chain	Res	Type
1	R	156	ASN
1	R	164	GLN
1	R	204	HIS
1	S	156	ASN
1	S	164	GLN
1	S	204	HIS
1	T	83	GLN
1	T	156	ASN
1	T	164	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	300	2	9,9,9	3.05	5 (55%)	10,12,12	2.20	5 (50%)
3	PGH	B	300	2	9,9,9	3.18	5 (55%)	10,12,12	2.64	6 (60%)
3	PGH	C	300	2	9,9,9	3.33	6 (66%)	10,12,12	2.22	6 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PGH	D	300	2	9,9,9	3.53	5 (55%)	10,12,12	2.44	5 (50%)
3	PGH	E	300	2	9,9,9	3.11	4 (44%)	10,12,12	2.89	6 (60%)
3	PGH	F	300	2	9,9,9	2.89	5 (55%)	10,12,12	2.48	4 (40%)
3	PGH	G	300	2	9,9,9	3.49	7 (77%)	10,12,12	2.15	5 (50%)
3	PGH	H	300	2	9,9,9	3.55	6 (66%)	10,12,12	2.20	6 (60%)
3	PGH	I	300	2	9,9,9	2.98	5 (55%)	10,12,12	2.86	4 (40%)
3	PGH	J	300	2	9,9,9	3.66	6 (66%)	10,12,12	2.96	7 (70%)
3	PGH	K	300	2	9,9,9	3.46	5 (55%)	10,12,12	2.89	5 (50%)
3	PGH	L	300	2	9,9,9	4.10	5 (55%)	10,12,12	2.58	7 (70%)
3	PGH	M	300	2	9,9,9	3.79	5 (55%)	10,12,12	2.75	7 (70%)
3	PGH	N	300	2	9,9,9	3.19	5 (55%)	10,12,12	2.89	6 (60%)
3	PGH	O	300	2	9,9,9	3.92	5 (55%)	10,12,12	2.91	4 (40%)
3	PGH	P	300	2	9,9,9	3.44	7 (77%)	10,12,12	2.38	4 (40%)
3	PGH	Q	300	2	9,9,9	3.35	5 (55%)	10,12,12	2.44	7 (70%)
3	PGH	R	300	2	9,9,9	3.34	5 (55%)	10,12,12	2.05	5 (50%)
3	PGH	S	300	2	9,9,9	3.00	5 (55%)	10,12,12	1.99	3 (30%)
3	PGH	T	300	2	9,9,9	3.72	7 (77%)	10,12,12	2.14	5 (50%)

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	A	300	2	-	0/8/8/8	0/0/0/0
3	PGH	B	300	2	-	0/8/8/8	0/0/0/0
3	PGH	C	300	2	-	0/8/8/8	0/0/0/0
3	PGH	D	300	2	-	0/8/8/8	0/0/0/0
3	PGH	E	300	2	-	0/8/8/8	0/0/0/0
3	PGH	F	300	2	-	0/8/8/8	0/0/0/0
3	PGH	G	300	2	-	0/8/8/8	0/0/0/0
3	PGH	H	300	2	-	0/8/8/8	0/0/0/0
3	PGH	I	300	2	-	0/8/8/8	0/0/0/0
3	PGH	J	300	2	-	0/8/8/8	0/0/0/0
3	PGH	K	300	2	-	0/8/8/8	0/0/0/0
3	PGH	L	300	2	-	0/8/8/8	0/0/0/0
3	PGH	M	300	2	-	0/8/8/8	0/0/0/0
3	PGH	N	300	2	-	0/8/8/8	0/0/0/0
3	PGH	O	300	2	-	0/8/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGH	P	300	2	-	0/8/8/8	0/0/0/0
3	PGH	Q	300	2	-	0/8/8/8	0/0/0/0
3	PGH	R	300	2	-	0/8/8/8	0/0/0/0
3	PGH	S	300	2	-	0/8/8/8	0/0/0/0
3	PGH	T	300	2	-	0/8/8/8	0/0/0/0

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	300	PGH	O1P-C2	-7.89	1.37	1.43
3	O	300	PGH	O1P-C2	-7.39	1.38	1.43
3	T	300	PGH	O1P-C2	-6.74	1.38	1.43
3	D	300	PGH	O1P-C2	-6.41	1.38	1.43
3	M	300	PGH	O1P-C2	-6.21	1.38	1.43
3	R	300	PGH	O1P-C2	-6.12	1.39	1.43
3	J	300	PGH	O1P-C2	-5.96	1.39	1.43
3	H	300	PGH	O1P-C2	-5.96	1.39	1.43
3	G	300	PGH	O1P-C2	-5.81	1.39	1.43
3	K	300	PGH	O1P-C2	-5.49	1.39	1.43
3	B	300	PGH	O1P-C2	-4.87	1.39	1.43
3	Q	300	PGH	O1P-C2	-4.77	1.39	1.43
3	N	300	PGH	O1P-C2	-3.64	1.40	1.43
3	S	300	PGH	O1P-C2	-3.62	1.40	1.43
3	C	300	PGH	O1P-C2	-3.57	1.40	1.43
3	F	300	PGH	O1P-C2	-3.56	1.40	1.43
3	P	300	PGH	O1P-C2	-3.27	1.40	1.43
3	A	300	PGH	O1P-C2	-3.22	1.40	1.43
3	G	300	PGH	C1-N2	-2.91	1.29	1.32
3	T	300	PGH	O2-N2	-2.81	1.34	1.39
3	H	300	PGH	O2-N2	-2.74	1.34	1.39
3	T	300	PGH	C1-N2	-2.65	1.29	1.32
3	G	300	PGH	O2-N2	-2.56	1.35	1.39
3	P	300	PGH	O2-N2	-2.49	1.35	1.39
3	C	300	PGH	O2-N2	-2.25	1.35	1.39
3	I	300	PGH	O2-N2	-2.19	1.35	1.39
3	J	300	PGH	C1-N2	-2.13	1.30	1.32
3	P	300	PGH	C1-N2	-2.04	1.30	1.32
3	D	300	PGH	P-O3P	2.15	1.62	1.54
3	B	300	PGH	P-O3P	2.24	1.62	1.54
3	Q	300	PGH	P-O3P	2.27	1.62	1.54
3	M	300	PGH	P-O3P	2.34	1.63	1.54
3	H	300	PGH	P-O3P	2.37	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	300	PGH	P-O3P	2.47	1.63	1.54
3	C	300	PGH	P-O3P	2.57	1.64	1.54
3	G	300	PGH	P-O2P	2.64	1.59	1.51
3	D	300	PGH	P-O2P	2.95	1.60	1.51
3	A	300	PGH	P-O3P	2.97	1.65	1.54
3	S	300	PGH	P-O3P	2.99	1.65	1.54
3	F	300	PGH	P-O3P	3.00	1.65	1.54
3	A	300	PGH	P-O4P	3.02	1.65	1.54
3	T	300	PGH	P-O2P	3.11	1.61	1.51
3	R	300	PGH	P-O3P	3.12	1.65	1.54
3	I	300	PGH	P-O3P	3.13	1.66	1.54
3	K	300	PGH	P-O3P	3.19	1.66	1.54
3	G	300	PGH	P-O3P	3.21	1.66	1.54
3	J	300	PGH	P-O3P	3.23	1.66	1.54
3	H	300	PGH	P-O2P	3.23	1.61	1.51
3	R	300	PGH	P-O4P	3.24	1.66	1.54
3	N	300	PGH	P-O3P	3.28	1.66	1.54
3	A	300	PGH	P-O2P	3.29	1.62	1.51
3	L	300	PGH	P-O3P	3.33	1.66	1.54
3	B	300	PGH	P-O4P	3.43	1.67	1.54
3	T	300	PGH	P-O3P	3.46	1.67	1.54
3	O	300	PGH	P-O3P	3.51	1.67	1.54
3	C	300	PGH	P-O2P	3.60	1.63	1.51
3	S	300	PGH	P-O4P	3.65	1.67	1.54
3	R	300	PGH	P-O2P	3.68	1.63	1.51
3	S	300	PGH	P-O2P	3.68	1.63	1.51
3	B	300	PGH	P-O2P	3.75	1.63	1.51
3	Q	300	PGH	P-O2P	3.78	1.63	1.51
3	F	300	PGH	P-O2P	3.79	1.63	1.51
3	K	300	PGH	P-O2P	3.80	1.63	1.51
3	P	300	PGH	P-O4P	3.84	1.68	1.54
3	L	300	PGH	P-O2P	3.86	1.63	1.51
3	P	300	PGH	P-O3P	3.90	1.68	1.54
3	H	300	PGH	P-O4P	3.96	1.68	1.54
3	M	300	PGH	P-O2P	3.97	1.64	1.51
3	J	300	PGH	P-O4P	3.97	1.69	1.54
3	N	300	PGH	P-O2P	3.99	1.64	1.51
3	T	300	PGH	P-O4P	3.99	1.69	1.54
3	O	300	PGH	P-O2P	3.99	1.64	1.51
3	I	300	PGH	P-O2P	4.03	1.64	1.51
3	F	300	PGH	P-O4P	4.05	1.69	1.54
3	E	300	PGH	P-O2P	4.07	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	300	PGH	P-O4P	4.08	1.69	1.54
3	D	300	PGH	P-O4P	4.08	1.69	1.54
3	G	300	PGH	P-O4P	4.15	1.69	1.54
3	Q	300	PGH	P-O4P	4.18	1.69	1.54
3	P	300	PGH	P-O2P	4.30	1.65	1.51
3	K	300	PGH	P-O4P	4.37	1.70	1.54
3	N	300	PGH	P-O4P	4.40	1.70	1.54
3	F	300	PGH	P-O1P	4.47	1.75	1.60
3	M	300	PGH	P-O4P	4.51	1.70	1.54
3	E	300	PGH	P-O4P	4.53	1.71	1.54
3	I	300	PGH	P-O4P	4.65	1.71	1.54
3	J	300	PGH	P-O2P	4.67	1.66	1.51
3	I	300	PGH	P-O1P	4.90	1.76	1.60
3	R	300	PGH	P-O1P	4.97	1.76	1.60
3	T	300	PGH	P-O1P	4.98	1.76	1.60
3	S	300	PGH	P-O1P	4.99	1.77	1.60
3	O	300	PGH	P-O4P	5.04	1.72	1.54
3	G	300	PGH	P-O1P	5.11	1.77	1.60
3	L	300	PGH	P-O4P	5.15	1.73	1.54
3	O	300	PGH	P-O1P	5.24	1.77	1.60
3	K	300	PGH	P-O1P	5.46	1.78	1.60
3	N	300	PGH	P-O1P	5.56	1.78	1.60
3	J	300	PGH	P-O1P	5.58	1.79	1.60
3	L	300	PGH	P-O1P	5.64	1.79	1.60
3	B	300	PGH	P-O1P	5.69	1.79	1.60
3	H	300	PGH	P-O1P	5.96	1.80	1.60
3	Q	300	PGH	P-O1P	6.02	1.80	1.60
3	P	300	PGH	P-O1P	6.02	1.80	1.60
3	E	300	PGH	P-O1P	6.11	1.80	1.60
3	A	300	PGH	P-O1P	6.22	1.81	1.60
3	D	300	PGH	P-O1P	6.26	1.81	1.60
3	C	300	PGH	P-O1P	6.73	1.82	1.60
3	M	300	PGH	P-O1P	6.83	1.83	1.60

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	300	PGH	O1P-P-O2P	-3.31	98.71	107.14
3	Q	300	PGH	O4P-P-O1P	-3.13	97.54	106.56
3	B	300	PGH	O1P-P-O2P	-3.01	99.47	107.14
3	H	300	PGH	O4P-P-O1P	-2.85	98.36	106.56
3	A	300	PGH	O1P-P-O2P	-2.82	99.98	107.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	300	PGH	O4P-P-O1P	-2.76	98.61	106.56
3	B	300	PGH	O4P-P-O1P	-2.69	98.81	106.56
3	O	300	PGH	O1P-P-O2P	-2.67	100.34	107.14
3	T	300	PGH	O1P-P-O2P	-2.66	100.37	107.14
3	I	300	PGH	O4P-P-O1P	-2.66	98.90	106.56
3	K	300	PGH	O4P-P-O1P	-2.66	98.90	106.56
3	E	300	PGH	O1P-P-O2P	-2.60	100.51	107.14
3	E	300	PGH	O4P-P-O2P	-2.60	102.22	110.58
3	J	300	PGH	O1P-P-O2P	-2.58	100.58	107.14
3	H	300	PGH	O1P-P-O2P	-2.58	100.59	107.14
3	E	300	PGH	O4P-P-O1P	-2.56	99.19	106.56
3	J	300	PGH	O4P-P-O2P	-2.56	102.34	110.58
3	N	300	PGH	O4P-P-O1P	-2.55	99.22	106.56
3	K	300	PGH	O1P-P-O2P	-2.51	100.75	107.14
3	M	300	PGH	O4P-P-O1P	-2.50	99.36	106.56
3	F	300	PGH	O4P-P-O1P	-2.40	99.65	106.56
3	T	300	PGH	O4P-P-O2P	-2.40	102.87	110.58
3	P	300	PGH	O4P-P-O1P	-2.38	99.72	106.56
3	R	300	PGH	O1P-P-O2P	-2.36	101.13	107.14
3	L	300	PGH	O4P-P-O1P	-2.32	99.87	106.56
3	D	300	PGH	O1P-P-O2P	-2.31	101.26	107.14
3	P	300	PGH	O1P-P-O2P	-2.30	101.30	107.14
3	Q	300	PGH	O4P-P-O2P	-2.28	103.24	110.58
3	M	300	PGH	O1P-P-O2P	-2.27	101.37	107.14
3	R	300	PGH	O4P-P-O1P	-2.24	100.10	106.56
3	M	300	PGH	O4P-P-O2P	-2.19	103.54	110.58
3	J	300	PGH	O4P-P-O1P	-2.17	100.32	106.56
3	N	300	PGH	O1P-P-O2P	-2.16	101.65	107.14
3	A	300	PGH	O4P-P-O1P	-2.16	100.36	106.56
3	S	300	PGH	O1P-P-O2P	-2.15	101.66	107.14
3	H	300	PGH	O4P-P-O2P	-2.12	103.74	110.58
3	F	300	PGH	O1P-P-O2P	-2.12	101.75	107.14
3	G	300	PGH	O4P-P-O1P	-2.10	100.52	106.56
3	C	300	PGH	O4P-P-O1P	-2.09	100.55	106.56
3	I	300	PGH	O1P-P-O2P	-2.08	101.86	107.14
3	L	300	PGH	O1P-P-O2P	-2.07	101.87	107.14
3	N	300	PGH	O4P-P-O2P	-2.07	103.93	110.58
3	Q	300	PGH	O1P-P-O2P	-2.04	101.95	107.14
3	G	300	PGH	O1P-P-O2P	-2.03	101.97	107.14
3	L	300	PGH	O4P-P-O2P	-2.02	104.07	110.58
3	B	300	PGH	O3P-P-O2P	2.00	117.03	110.58
3	K	300	PGH	O3P-P-O2P	2.06	117.22	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	300	PGH	O1-C1-N2	2.07	125.98	123.53
3	C	300	PGH	O4P-P-O3P	2.10	115.37	107.38
3	R	300	PGH	O4P-P-O3P	2.13	115.49	107.38
3	M	300	PGH	O3P-P-O2P	2.13	117.45	110.58
3	J	300	PGH	O3P-P-O2P	2.19	117.63	110.58
3	Q	300	PGH	O4P-P-O3P	2.22	115.82	107.38
3	L	300	PGH	O3P-P-O2P	2.22	117.74	110.58
3	J	300	PGH	O4P-P-O3P	2.22	115.85	107.38
3	G	300	PGH	O3P-P-O2P	2.23	117.77	110.58
3	N	300	PGH	O3P-P-O2P	2.24	117.78	110.58
3	L	300	PGH	O2-N2-C1	2.38	123.16	119.56
3	Q	300	PGH	O3P-P-O2P	2.38	118.24	110.58
3	A	300	PGH	O3P-P-O2P	2.48	118.56	110.58
3	M	300	PGH	O4P-P-O3P	2.49	116.85	107.38
3	B	300	PGH	O4P-P-O3P	2.49	116.86	107.38
3	T	300	PGH	O1-C1-N2	2.59	126.60	123.53
3	T	300	PGH	O3P-P-O2P	2.70	119.28	110.58
3	O	300	PGH	O3P-P-O2P	2.77	119.48	110.58
3	C	300	PGH	O3P-P-O1P	2.84	114.74	106.56
3	S	300	PGH	O1-C1-N2	2.85	126.90	123.53
3	C	300	PGH	O3P-P-O2P	2.86	119.78	110.58
3	C	300	PGH	O1-C1-N2	2.88	126.94	123.53
3	D	300	PGH	O3P-P-O1P	2.91	114.94	106.56
3	A	300	PGH	O3P-P-O1P	2.93	115.00	106.56
3	E	300	PGH	O3P-P-O2P	2.97	120.12	110.58
3	R	300	PGH	O1-C1-N2	3.08	127.17	123.53
3	D	300	PGH	O3P-P-O2P	3.09	120.53	110.58
3	M	300	PGH	O3P-P-O1P	3.13	115.58	106.56
3	H	300	PGH	O3P-P-O1P	3.19	115.74	106.56
3	H	300	PGH	O3P-P-O2P	3.28	121.15	110.58
3	G	300	PGH	O1-C1-N2	3.32	127.46	123.53
3	G	300	PGH	O3P-P-O1P	3.36	116.23	106.56
3	R	300	PGH	O3P-P-O1P	3.45	116.51	106.56
3	T	300	PGH	O3P-P-O1P	3.54	116.75	106.56
3	Q	300	PGH	O3P-P-O1P	3.62	117.00	106.56
3	E	300	PGH	O3P-P-O1P	3.67	117.14	106.56
3	Q	300	PGH	O1-C1-N2	3.72	127.93	123.53
3	A	300	PGH	O1-C1-N2	3.72	127.94	123.53
3	J	300	PGH	O3P-P-O1P	3.74	117.32	106.56
3	B	300	PGH	O3P-P-O1P	3.74	117.32	106.56
3	L	300	PGH	O3P-P-O1P	3.95	117.95	106.56
3	S	300	PGH	O3P-P-O1P	4.00	118.07	106.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	300	PGH	O3P-P-O1P	4.01	118.11	106.56
3	N	300	PGH	O3P-P-O1P	4.08	118.30	106.56
3	F	300	PGH	O3P-P-O1P	4.09	118.34	106.56
3	O	300	PGH	O3P-P-O1P	4.11	118.40	106.56
3	D	300	PGH	O1-C1-N2	4.37	128.70	123.53
3	K	300	PGH	O3P-P-O1P	4.41	119.26	106.56
3	P	300	PGH	O1-C1-N2	4.45	128.79	123.53
3	I	300	PGH	O3P-P-O1P	4.62	119.86	106.56
3	L	300	PGH	O1-C1-N2	4.75	129.15	123.53
3	F	300	PGH	O1-C1-N2	4.76	129.17	123.53
3	B	300	PGH	O1-C1-N2	4.83	129.25	123.53
3	M	300	PGH	O1-C1-N2	5.84	130.44	123.53
3	E	300	PGH	O1-C1-N2	5.90	130.50	123.53
3	K	300	PGH	O1-C1-N2	6.07	130.71	123.53
3	I	300	PGH	O1-C1-N2	6.13	130.78	123.53
3	N	300	PGH	O1-C1-N2	6.34	131.02	123.53
3	J	300	PGH	O1-C1-N2	6.34	131.03	123.53
3	O	300	PGH	O1-C1-N2	6.36	131.06	123.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	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, 95^{th} 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%)	-0.13	3 (1%) 82 83	23, 37, 60, 84	0
1	B	274/274 (100%)	-0.19	1 (0%) 93 94	23, 37, 60, 84	0
1	C	274/274 (100%)	-0.18	2 (0%) 89 90	23, 37, 60, 84	0
1	D	274/274 (100%)	-0.00	5 (1%) 71 72	23, 37, 60, 84	0
1	E	274/274 (100%)	-0.24	1 (0%) 93 94	23, 37, 60, 84	0
1	F	274/274 (100%)	-0.22	0 100 100	23, 37, 60, 84	0
1	G	274/274 (100%)	-0.15	3 (1%) 82 83	23, 37, 60, 84	0
1	H	274/274 (100%)	-0.05	3 (1%) 82 83	23, 37, 60, 84	0
1	I	274/274 (100%)	-0.00	11 (4%) 42 41	23, 37, 60, 84	0
1	J	274/274 (100%)	0.19	21 (7%) 16 14	23, 37, 60, 84	0
1	K	274/274 (100%)	0.56	34 (12%) 5 4	23, 37, 60, 84	0
1	L	274/274 (100%)	0.43	21 (7%) 16 14	23, 37, 60, 84	0
1	M	274/274 (100%)	-0.29	7 (2%) 59 59	23, 37, 60, 84	0
1	N	274/274 (100%)	0.11	14 (5%) 32 30	23, 37, 60, 84	0
1	O	274/274 (100%)	0.58	38 (13%) 4 3	23, 37, 60, 84	0
1	P	274/274 (100%)	0.30	21 (7%) 16 14	23, 37, 60, 84	0
1	Q	274/274 (100%)	-0.10	3 (1%) 82 83	23, 37, 60, 84	0
1	R	274/274 (100%)	-0.04	0 100 100	23, 37, 60, 84	0
1	S	274/274 (100%)	-0.12	2 (0%) 89 90	23, 37, 60, 84	0
1	T	274/274 (100%)	-0.13	1 (0%) 93 94	23, 37, 60, 84	0
All	All	5480/5480 (100%)	0.02	191 (3%) 48 48	23, 37, 60, 84	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	51	GLN	5.7
1	D	51	GLN	5.7
1	O	274	LEU	5.6
1	Q	51	GLN	5.0
1	M	274	LEU	4.9
1	O	273	ALA	4.7
1	M	51	GLN	4.7
1	O	160	VAL	4.5
1	D	274	LEU	4.3
1	K	51	GLN	4.3
1	K	63	PRO	4.2
1	O	52	GLN	4.2
1	K	273	ALA	4.1
1	O	51	GLN	4.1
1	A	51	GLN	4.0
1	J	64	LEU	4.0
1	L	261	LYS	3.8
1	H	63	PRO	3.8
1	P	99	GLY	3.7
1	I	274	LEU	3.7
1	J	101	GLY	3.6
1	O	133	ASN	3.6
1	K	160	VAL	3.6
1	O	159	ALA	3.6
1	I	273	ALA	3.5
1	K	257	ILE	3.5
1	O	100	ALA	3.5
1	K	261	LYS	3.5
1	B	51	GLN	3.5
1	M	273	ALA	3.5
1	O	69	PRO	3.4
1	C	51	GLN	3.4
1	K	254	GLU	3.4
1	K	97	SER	3.4
1	J	274	LEU	3.3
1	O	53	PRO	3.3
1	M	272	LEU	3.2
1	K	59	SER	3.2
1	K	98	ASP	3.2
1	L	272	LEU	3.2
1	O	39	ASP	3.2
1	K	66	ALA	3.2
1	P	100	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	55	TYR	3.1
1	L	35	LEU	3.1
1	O	42	ILE	3.1
1	J	99	GLY	3.1
1	L	274	LEU	3.1
1	K	274	LEU	3.0
1	N	274	LEU	3.0
1	O	98	ASP	3.0
1	I	50	HIS	3.0
1	O	253	ARG	3.0
1	K	268	LEU	2.9
1	L	269	ALA	2.9
1	P	202	GLN	2.9
1	M	50	HIS	2.9
1	D	273	ALA	2.9
1	K	269	ALA	2.9
1	O	65	LEU	2.9
1	D	52	GLN	2.8
1	K	272	LEU	2.8
1	I	52	GLN	2.8
1	N	61	PRO	2.8
1	O	257	ILE	2.8
1	P	63	PRO	2.8
1	I	268	LEU	2.8
1	J	57	PRO	2.8
1	E	51	GLN	2.7
1	O	96	ASP	2.7
1	P	97	SER	2.7
1	O	270	SER	2.7
1	J	98	ASP	2.6
1	O	63	PRO	2.6
1	N	65	LEU	2.6
1	P	60	GLN	2.6
1	J	67	ASN	2.6
1	P	98	ASP	2.6
1	K	262	ARG	2.6
1	K	266	THR	2.6
1	I	270	SER	2.6
1	L	40	ALA	2.6
1	K	46	HIS	2.6
1	H	155	GLU	2.6
1	P	56	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	N	64	LEU	2.6
1	O	155	GLU	2.6
1	O	203	LYS	2.6
1	K	203	LYS	2.5
1	O	135	LYS	2.5
1	P	101	GLY	2.5
1	K	187	VAL	2.5
1	K	271	ALA	2.5
1	L	257	ILE	2.5
1	S	199	GLN	2.5
1	O	101	GLY	2.5
1	L	129	ILE	2.5
1	O	64	LEU	2.5
1	O	67	ASN	2.5
1	P	55	TYR	2.5
1	S	203	LYS	2.5
1	L	133	ASN	2.5
1	L	251	ILE	2.5
1	L	258	ALA	2.5
1	N	40	ALA	2.5
1	O	271	ALA	2.5
1	N	52	GLN	2.5
1	O	130	LYS	2.4
1	N	273	ALA	2.4
1	O	62	MET	2.4
1	P	191	ASP	2.4
1	K	270	SER	2.4
1	L	254	GLU	2.4
1	Q	254	GLU	2.4
1	O	58	LEU	2.4
1	N	98	ASP	2.4
1	K	267	PRO	2.4
1	N	51	GLN	2.4
1	O	254	GLU	2.3
1	P	268	LEU	2.3
1	M	52	GLN	2.3
1	J	111	GLU	2.3
1	G	274	LEU	2.3
1	L	135	LYS	2.3
1	P	64	LEU	2.3
1	A	50	HIS	2.3
1	C	52	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	269	ALA	2.3
1	L	268	LEU	2.3
1	A	52	GLN	2.3
1	J	273	ALA	2.3
1	L	101	GLY	2.3
1	K	106	TRP	2.3
1	K	264	GLY	2.3
1	K	52	GLN	2.3
1	J	158	THR	2.3
1	L	52	GLN	2.3
1	O	61	PRO	2.3
1	O	46	HIS	2.3
1	K	166	TRP	2.3
1	L	248	LYS	2.2
1	P	248	LYS	2.2
1	P	257	ILE	2.2
1	J	61	PRO	2.2
1	J	184	PRO	2.2
1	N	63	PRO	2.2
1	I	269	ALA	2.2
1	N	43	ALA	2.2
1	P	65	LEU	2.2
1	I	271	ALA	2.2
1	L	273	ALA	2.2
1	T	100	ALA	2.2
1	K	250	THR	2.2
1	K	163	ARG	2.2
1	O	55	TYR	2.2
1	P	67	ASN	2.2
1	D	50	HIS	2.2
1	J	58	LEU	2.2
1	O	202	GLN	2.2
1	G	261	LYS	2.2
1	K	189	GLY	2.2
1	N	49	PHE	2.2
1	O	95	VAL	2.2
1	G	52	GLN	2.1
1	P	62	MET	2.1
1	I	272	LEU	2.1
1	J	133	ASN	2.1
1	O	66	ALA	2.1
1	M	253	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	P	133	ASN	2.1
1	H	191	ASP	2.1
1	N	100	ALA	2.1
1	P	66	ALA	2.1
1	O	127	GLU	2.1
1	K	195	GLN	2.1
1	J	159	ALA	2.1
1	K	251	ILE	2.1
1	K	101	GLY	2.1
1	Q	52	GLN	2.0
1	L	130	LYS	2.0
1	N	101	GLY	2.0
1	J	102	TYR	2.0
1	J	156	ASN	2.0
1	K	265	VAL	2.0
1	L	266	THR	2.0
1	P	69	PRO	2.0
1	O	195	GLN	2.0
1	I	248	LYS	2.0
1	J	130	LYS	2.0
1	L	256	LEU	2.0
1	J	63	PRO	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	PGH	G	300	10/10	0.97	0.17	2.06	50,52,53,54	0
3	PGH	C	300	10/10	0.97	0.20	1.35	50,52,53,54	0
3	PGH	A	300	10/10	0.98	0.18	0.95	50,52,53,54	0
3	PGH	E	300	10/10	0.96	0.16	0.71	50,52,53,54	0
3	PGH	I	300	10/10	0.96	0.14	0.71	50,52,53,54	0
3	PGH	S	300	10/10	0.98	0.16	0.67	50,52,53,54	0
3	PGH	T	300	10/10	0.97	0.17	0.58	50,52,53,54	0
3	PGH	L	300	10/10	0.94	0.16	0.53	50,52,53,54	0
3	PGH	B	300	10/10	0.98	0.15	0.31	50,52,53,54	0
3	PGH	P	300	10/10	0.96	0.14	0.21	50,52,53,54	0
3	PGH	M	300	10/10	0.96	0.13	0.14	50,52,53,54	0
3	PGH	F	300	10/10	0.97	0.16	0.14	50,52,53,54	0
3	PGH	N	300	10/10	0.96	0.13	0.11	50,52,53,54	0
3	PGH	O	300	10/10	0.95	0.15	0.10	50,52,53,54	0
3	PGH	H	300	10/10	0.98	0.16	-0.00	50,52,53,54	0
3	PGH	D	300	10/10	0.98	0.18	-0.01	50,52,53,54	0
3	PGH	J	300	10/10	0.96	0.13	-0.08	50,52,53,54	0
3	PGH	Q	300	10/10	0.97	0.17	-0.13	50,52,53,54	0
3	PGH	R	300	10/10	0.99	0.16	-0.23	50,52,53,54	0
3	PGH	K	300	10/10	0.95	0.14	-0.42	50,52,53,54	0
2	ZN	C	275	1/1	1.00	0.17	-1.01	32,32,32,32	0
2	ZN	R	275	1/1	1.00	0.13	-2.34	32,32,32,32	0
2	ZN	S	275	1/1	0.98	0.11	-2.49	33,33,33,33	0
2	ZN	D	275	1/1	1.00	0.14	-3.83	32,32,32,32	0
2	ZN	J	275	1/1	0.98	0.03	-3.88	35,35,35,35	0
2	ZN	I	275	1/1	0.99	0.04	-4.14	34,34,34,34	0
2	ZN	O	275	1/1	0.97	0.03	-4.45	35,35,35,35	0
2	ZN	K	275	1/1	0.96	0.04	-5.92	35,35,35,35	0
2	ZN	T	275	1/1	0.99	0.14	-	33,33,33,33	0
2	ZN	N	275	1/1	0.98	0.03	-	35,35,35,35	0
2	ZN	M	275	1/1	0.99	0.04	-	33,33,33,33	0
2	ZN	P	275	1/1	0.99	0.05	-	34,34,34,34	0
2	ZN	H	275	1/1	0.99	0.13	-	32,32,32,32	0
2	ZN	Q	275	1/1	1.00	0.14	-	32,32,32,32	0
2	ZN	L	275	1/1	0.99	0.04	-	35,35,35,35	0
2	ZN	B	275	1/1	1.00	0.12	-	32,32,32,32	0
2	ZN	G	275	1/1	0.99	0.08	-	34,34,34,34	0
2	ZN	A	275	1/1	1.00	0.16	-	32,32,32,32	0
2	ZN	F	275	1/1	0.99	0.13	-	34,34,34,34	0
2	ZN	E	275	1/1	0.99	0.11	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.