



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:24 AM GMT

PDB ID : 3AI7  
Title : Crystal Structure of Bifidobacterium Longum Phosphoketolase  
Authors : Takahashi, K.; Tagami, U.; Shimba, N.; Kashiwagi, T.; Ishikawa, K.; Suzuki, E.  
Deposited on : 2010-05-10  
Resolution : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

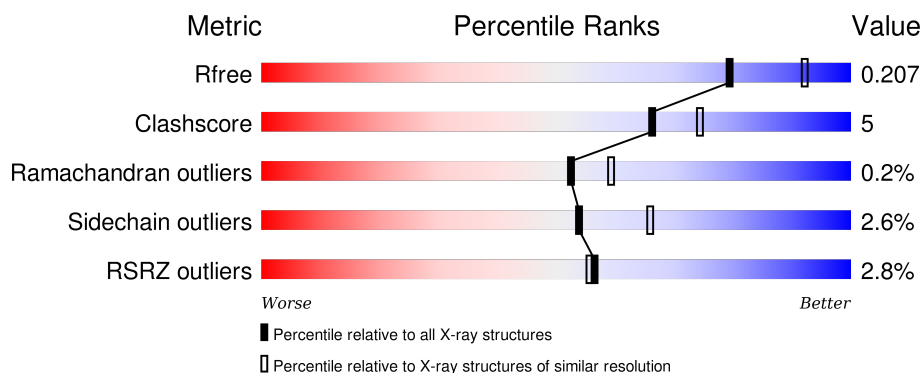
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	831	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	B	831	<div> <div>2%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
1	C	831	<div> <div>3%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	D	831	<div> <div>2%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
1	E	831	<div> <div>4%</div> <div>87%</div> <div>9%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	831	<div><div></div><div>4%</div><div>84%</div><div>12%</div><div>••</div></div>
1	G	831	<div><div></div><div>2%</div><div>88%</div><div>9%</div><div>•</div></div>
1	H	831	<div><div></div><div>2%</div><div>86%</div><div>11%</div><div>••</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 56952 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 Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	B	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	C	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	D	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	E	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	F	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	G	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			
1	H	813	Total	C	N	O	S	0	0	0
			6460	4101	1102	1238	19			

There are 48 discrepancies between the modelled and reference sequences:

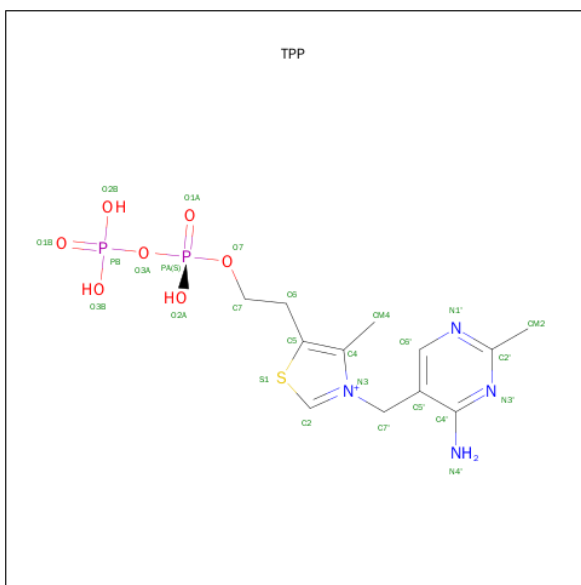
Chain	Residue	Modelled	Actual	Comment	Reference
A	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
A	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
A	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
A	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
A	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
A	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
B	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
C	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
C	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
C	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
C	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
C	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
D	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
E	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
F	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
G	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	826	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	827	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	828	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	829	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	830	HIS	-	EXPRESSION TAG	UNP Q6R2Q7
H	831	HIS	-	EXPRESSION TAG	UNP Q6R2Q7

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0
3	C	1	Total 1	Ca 1	0	0
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

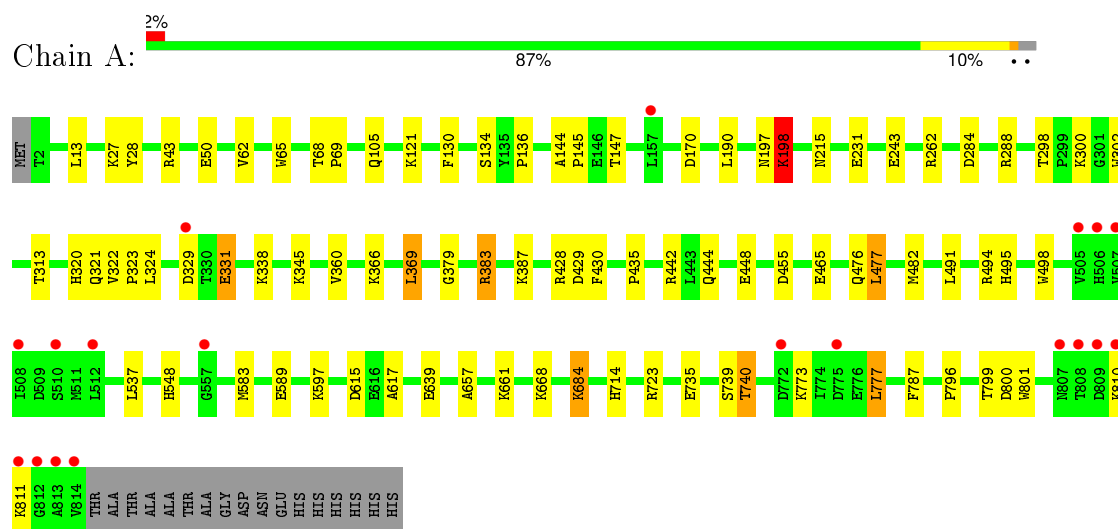
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	685	Total 685	O 685	0	0
4	B	670	Total 670	O 670	0	0
4	C	628	Total 628	O 628	0	0
4	D	621	Total 621	O 621	0	0
4	E	653	Total 653	O 653	0	0
4	F	590	Total 590	O 590	0	0
4	G	620	Total 620	O 620	0	0
4	H	589	Total 589	O 589	0	0

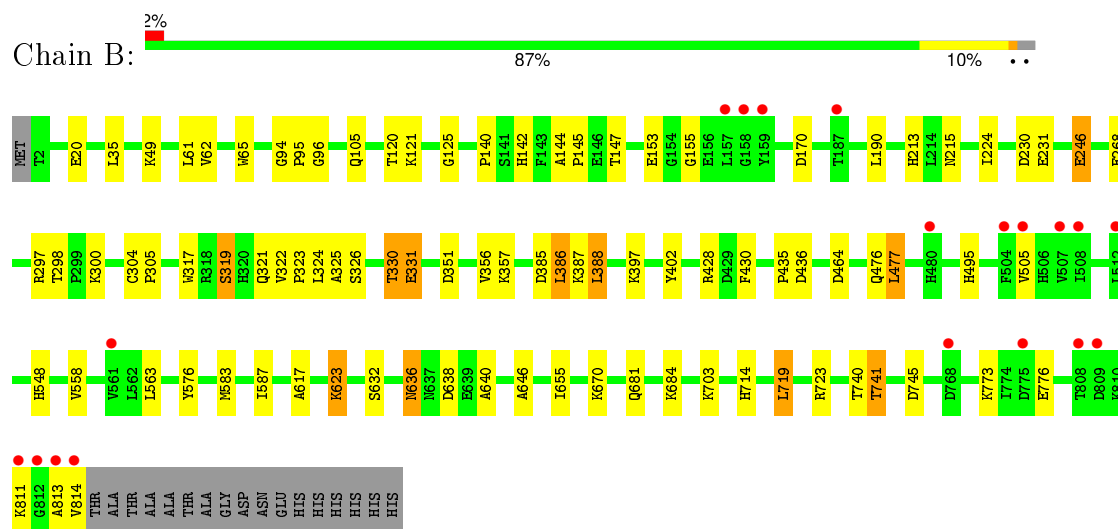
### 3 Residue-property plots [i](#)

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.

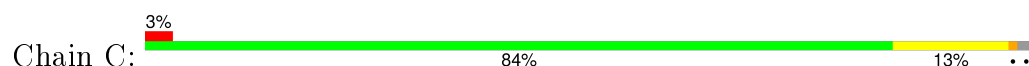
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



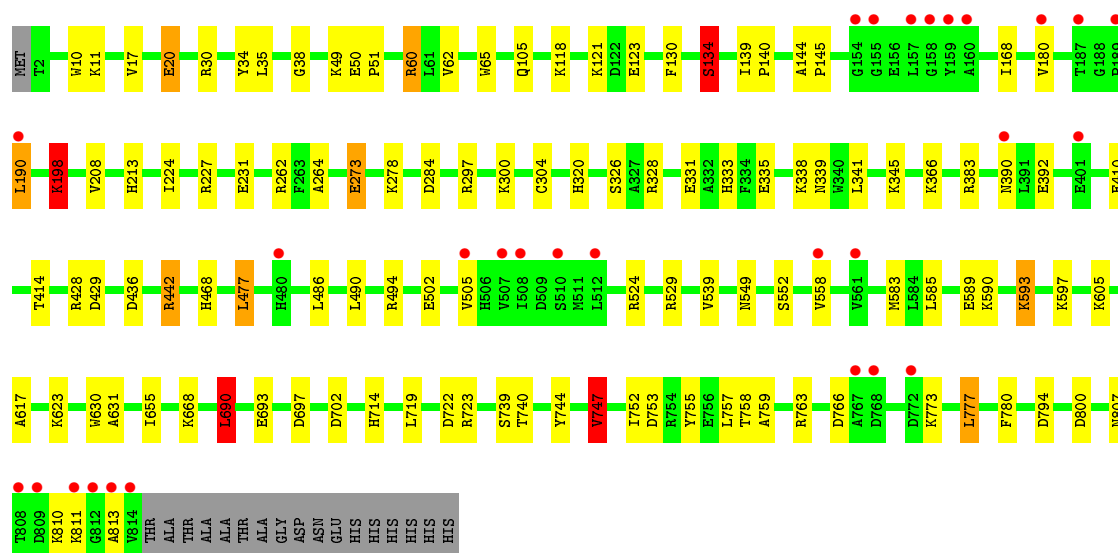
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



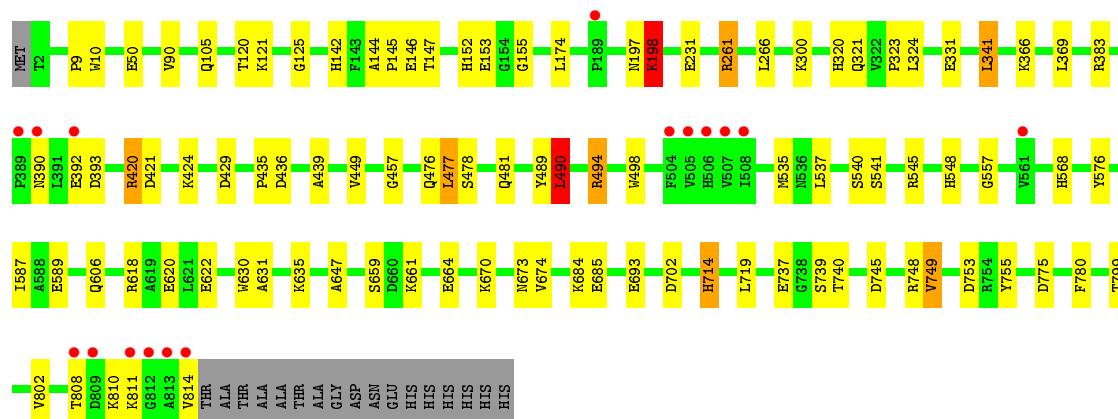
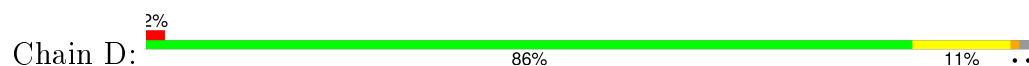
- Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



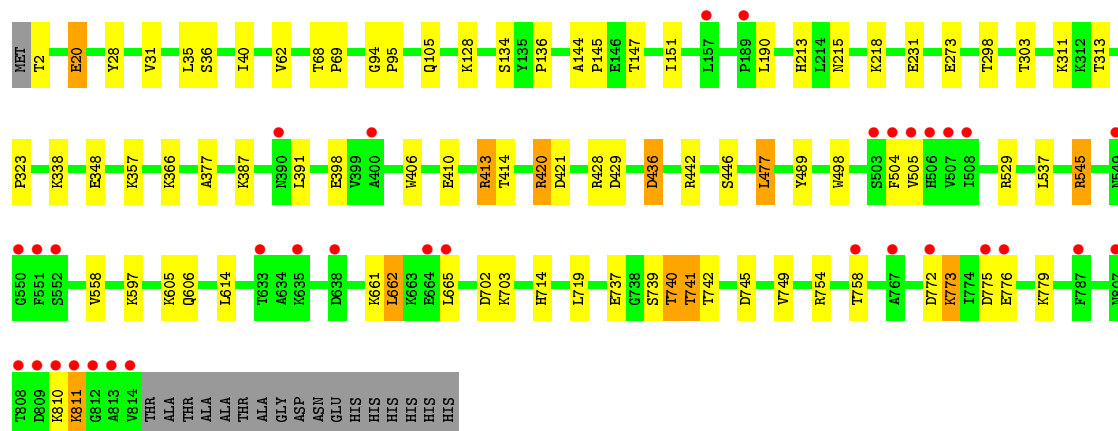
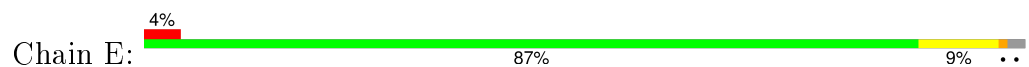




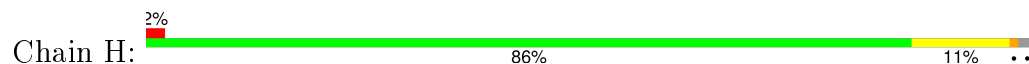
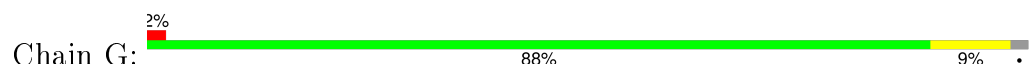
• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase

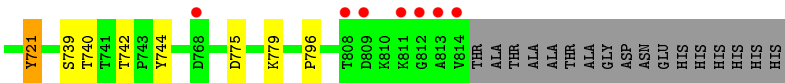


• Molecule 1: Xylulose-5-phosphate/fructose-6-phosphate phosphoketolase



Chain F:  4% 84% 12% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.26Å 184.41Å 157.44Å 90.00° 97.31° 90.00°	Depositor
Resolution (Å)	47.87 – 2.20 47.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.87-2.20) 98.9 (47.87-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.147 , 0.206 0.149 , 0.207	Depositor DCC
$R_{free}$ test set	20230 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 401973 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	56952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: CA, TPP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.17	8/6637 (0.1%)	0.95	12/9025 (0.1%)
1	B	1.14	5/6637 (0.1%)	0.96	9/9025 (0.1%)
1	C	1.15	9/6637 (0.1%)	0.98	26/9025 (0.3%)
1	D	1.12	5/6637 (0.1%)	0.96	12/9025 (0.1%)
1	E	1.10	5/6637 (0.1%)	0.95	10/9025 (0.1%)
1	F	1.09	2/6637 (0.0%)	0.92	9/9025 (0.1%)
1	G	1.12	4/6637 (0.1%)	0.92	10/9025 (0.1%)
1	H	1.09	7/6637 (0.1%)	0.90	5/9025 (0.1%)
All	All	1.12	45/53096 (0.1%)	0.94	93/72200 (0.1%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	231	GLU	CG-CD	8.11	1.64	1.51
1	A	231	GLU	CG-CD	7.66	1.63	1.51
1	H	744	TYR	CE1-CZ	7.04	1.47	1.38
1	C	231	GLU	CG-CD	6.99	1.62	1.51
1	G	362	ALA	CA-CB	6.71	1.66	1.52
1	C	123	GLU	CB-CG	6.52	1.64	1.52
1	C	60	ARG	CG-CD	6.15	1.67	1.51
1	A	589	GLU	CG-CD	6.15	1.61	1.51
1	C	123	GLU	CG-CD	6.13	1.61	1.51
1	A	448	GLU	CG-CD	5.87	1.60	1.51
1	G	231	GLU	CG-CD	5.86	1.60	1.51
1	D	231	GLU	CG-CD	5.79	1.60	1.51
1	A	735	GLU	CB-CG	-5.78	1.41	1.52
1	D	261	ARG	CG-CD	5.72	1.66	1.51
1	H	721	TYR	CE2-CZ	5.71	1.46	1.38
1	F	449	VAL	CB-CG1	-5.66	1.41	1.52
1	B	246	GLU	CB-CG	5.63	1.62	1.52
1	C	702	ASP	CB-CG	5.57	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	331	GLU	CG-CD	5.57	1.60	1.51
1	H	245	TYR	CD1-CE1	5.53	1.47	1.39
1	C	331	GLU	CG-CD	5.53	1.60	1.51
1	H	290	PHE	CE2-CZ	5.51	1.47	1.37
1	C	273	GLU	CG-CD	5.49	1.60	1.51
1	E	504	PHE	CE1-CZ	5.40	1.47	1.37
1	E	28	TYR	CD2-CE2	5.38	1.47	1.39
1	B	317	TRP	CE3-CZ3	5.38	1.47	1.38
1	B	331	GLU	CG-CD	5.30	1.59	1.51
1	H	331	GLU	CG-CD	5.30	1.59	1.51
1	G	112	TYR	CD2-CE2	-5.29	1.31	1.39
1	B	319	SER	CB-OG	5.27	1.49	1.42
1	F	32	ALA	CA-CB	5.26	1.63	1.52
1	H	20	GLU	CG-CD	5.23	1.59	1.51
1	A	243	GLU	CG-CD	5.23	1.59	1.51
1	D	685	GLU	CG-CD	5.23	1.59	1.51
1	C	747	VAL	CB-CG2	-5.21	1.42	1.52
1	A	130	PHE	CE1-CZ	5.16	1.47	1.37
1	A	787	PHE	CE2-CZ	5.15	1.47	1.37
1	D	366	LYS	CD-CE	5.15	1.64	1.51
1	D	439	ALA	CA-CB	5.15	1.63	1.52
1	C	20	GLU	CG-CD	5.11	1.59	1.51
1	G	749	VAL	CB-CG2	5.09	1.63	1.52
1	B	268	GLU	CD-OE2	5.03	1.31	1.25
1	H	231	GLU	CG-CD	5.03	1.59	1.51
1	E	489	TYR	CD1-CE1	5.02	1.46	1.39
1	E	20	GLU	CG-CD	5.02	1.59	1.51

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	B	297	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	383	ARG	NE-CZ-NH1	-8.27	116.16	120.30
1	E	338	LYS	CD-CE-NZ	-8.15	92.96	111.70
1	A	615	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	777	LEU	CB-CG-CD1	7.40	123.58	111.00
1	C	383	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	F	383	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	D	420	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	E	413	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	D	393	ASP	CB-CG-OD2	-7.23	111.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	358	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	F	297	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	436	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	C	593	LYS	CD-CE-NZ	-7.04	95.50	111.70
1	F	318	ARG	NE-CZ-NH1	-6.99	116.81	120.30
1	A	198	LYS	CD-CE-NZ	6.95	127.68	111.70
1	D	198	LYS	CD-CE-NZ	6.85	127.45	111.70
1	G	30	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	G	358	ASP	CB-CG-OD1	6.70	124.33	118.30
1	E	436	ASP	CB-CG-OD2	6.64	124.27	118.30
1	C	198	LYS	CD-CE-NZ	6.62	126.93	111.70
1	C	719	LEU	CB-CG-CD2	-6.51	99.94	111.00
1	C	719	LEU	CA-CB-CG	6.50	130.26	115.30
1	H	109	ASP	CB-CG-OD1	6.49	124.14	118.30
1	D	341	LEU	CA-CB-CG	6.48	130.21	115.30
1	C	383	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	702	ASP	CB-CG-OD1	6.44	124.09	118.30
1	F	702	ASP	CB-CG-OD1	6.42	124.08	118.30
1	H	225	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	F	477	LEU	CB-CG-CD1	6.38	121.85	111.00
1	E	545	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	F	43	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	284	ASP	CB-CG-OD1	6.23	123.91	118.30
1	E	719	LEU	CB-CG-CD2	-6.22	100.42	111.00
1	D	477	LEU	CB-CG-CD1	6.22	121.58	111.00
1	D	420	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	D	393	ASP	CB-CG-OD1	6.09	123.78	118.30
1	E	529	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	C	529	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	G	284	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	C	766	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	482	MET	CG-SD-CE	5.95	109.72	100.20
1	C	262	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	436	ASP	CB-CG-OD1	5.93	123.64	118.30
1	H	420	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	30	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	49	LYS	CD-CE-NZ	-5.82	98.33	111.70
1	F	109	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	464	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	284	ASP	CB-CG-OD1	5.76	123.48	118.30
1	G	719	LEU	CA-CB-CG	5.73	128.48	115.30
1	G	702	ASP	CB-CG-OD1	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	490	LEU	CB-CG-CD1	5.72	120.72	111.00
1	A	723	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	C	134	SER	CB-CA-C	5.70	120.93	110.10
1	G	558	VAL	CB-CA-C	-5.69	100.58	111.40
1	D	383	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	H	420	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	719	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	C	690	LEU	CA-CB-CG	5.60	128.19	115.30
1	B	388	LEU	CB-CG-CD1	5.60	120.52	111.00
1	B	385	ASP	CB-CG-OD1	5.57	123.32	118.30
1	A	369	LEU	CB-CG-CD1	5.55	120.43	111.00
1	C	436	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	262	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	H	715	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	297	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	477	LEU	CB-CG-CD1	5.45	120.27	111.00
1	G	383	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	428	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	E	436	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	E	702	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	328	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	C	297	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	386	LEU	CB-CG-CD1	5.27	119.96	111.00
1	C	722	ASP	CB-CG-OD2	5.25	123.02	118.30
1	G	30	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	329	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	366	LYS	CD-CE-NZ	5.24	123.74	111.70
1	C	800	ASP	CB-CG-OD1	5.20	122.98	118.30
1	F	549	ASN	N-CA-C	5.20	125.03	111.00
1	D	719	LEU	CA-CB-CG	5.19	127.23	115.30
1	C	549	ASN	N-CA-C	5.18	125.00	111.00
1	E	420	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	E	529	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	A	383	ARG	CG-CD-NE	-5.13	101.02	111.80
1	B	719	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	766	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	G	128	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	B	324	LEU	N-CA-C	-5.04	97.39	111.00
1	C	747	VAL	CB-CA-C	5.02	120.93	111.40
1	A	324	LEU	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.



There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6460	0	6155	58	0
1	B	6460	0	6155	59	0
1	C	6460	0	6155	68	0
1	D	6460	0	6155	52	0
1	E	6460	0	6155	63	0
1	F	6460	0	6155	82	0
1	G	6460	0	6155	65	0
1	H	6460	0	6155	67	0
2	A	26	0	16	4	0
2	B	26	0	16	3	0
2	C	26	0	16	2	0
2	D	26	0	16	2	0
2	E	26	0	16	3	0
2	F	26	0	16	3	0
2	G	26	0	16	1	0
2	H	26	0	16	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	685	0	0	26	0
4	B	670	0	0	17	0
4	C	628	0	0	29	1
4	D	621	0	0	18	0
4	E	653	0	0	23	1
4	F	590	0	0	18	0
4	G	620	0	0	21	0
4	H	589	0	0	29	0
All	All	56952	0	49368	500	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (500) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:LYS:HD3	4:A:3464:HOH:O	1.40	1.20
1:H:684:LYS:HD3	4:H:921:HOH:O	1.47	1.14
1:G:558:VAL:HG23	4:G:951:HOH:O	1.48	1.13
1:E:810:LYS:HG3	4:E:4920:HOH:O	1.48	1.11
1:F:428:ARG:HH11	1:F:428:ARG:HG2	0.99	1.08
1:G:390:ASN:HB2	4:G:3444:HOH:O	1.53	1.05
1:B:741:THR:HG21	1:B:745:ASP:OD2	1.57	1.04
1:H:597:LYS:HD2	4:H:2774:HOH:O	1.58	1.04
1:G:638:ASP:HB3	4:G:2809:HOH:O	1.57	1.02
1:D:331:GLU:HG2	4:D:3432:HOH:O	1.58	1.02
1:C:273:GLU:HG2	4:C:915:HOH:O	1.59	1.01
1:F:465:GLU:HG3	4:F:4832:HOH:O	1.57	1.00
1:G:353:ASN:HB2	4:G:4087:HOH:O	1.63	0.97
1:E:741:THR:HG22	1:F:136:PRO:HA	1.48	0.94
1:G:700:THR:CG2	1:G:703:LYS:H	1.81	0.94
1:H:465:GLU:HG3	4:H:909:HOH:O	1.67	0.94
1:E:273:GLU:HG2	4:E:915:HOH:O	1.67	0.94
1:G:699:PHE:O	1:G:700:THR:HB	1.63	0.94
1:E:737:GLU:HB3	1:E:749:VAL:HG12	1.50	0.92
1:F:428:ARG:HH11	1:F:428:ARG:CG	1.83	0.90
1:A:197:ASN:OD1	1:A:198:LYS:HE3	1.73	0.89
1:A:321:GLN:HG2	4:A:906:HOH:O	1.71	0.89
1:F:428:ARG:NH1	1:F:428:ARG:HG2	1.78	0.89
1:B:623:LYS:HB2	4:B:1665:HOH:O	1.74	0.88
1:H:60:ARG:HD2	4:H:880:HOH:O	1.73	0.88
1:E:703:LYS:HE2	4:E:2254:HOH:O	1.74	0.87
1:H:273:GLU:HG2	4:H:4819:HOH:O	1.73	0.87
4:E:2490:HOH:O	1:F:714:HIS:HE1	1.56	0.86
1:F:353:ASN:HB2	4:F:2567:HOH:O	1.75	0.86
1:E:62:VAL:HG13	1:F:548:HIS:HA	1.59	0.85
1:B:49:LYS:HE2	4:B:935:HOH:O	1.76	0.85
1:D:197:ASN:OD1	1:D:198:LYS:HE3	1.77	0.84
1:D:144:ALA:HB1	1:D:145:PRO:HD2	1.59	0.84
1:C:390:ASN:HB2	4:C:3986:HOH:O	1.78	0.83
1:D:618:ARG:HD3	4:D:933:HOH:O	1.78	0.82
1:C:590:LYS:HE3	4:C:1554:HOH:O	1.79	0.82
1:A:597:LYS:HD3	4:A:2344:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:306:LYS:HE2	4:F:4993:HOH:O	1.78	0.82
1:E:413:ARG:HH11	1:E:442:ARG:HD3	1.43	0.80
1:B:397:LYS:HE2	4:B:949:HOH:O	1.82	0.79
1:H:55:GLU:HG2	4:H:5025:HOH:O	1.82	0.79
1:H:420:ARG:HD2	1:H:421:ASP:OD1	1.82	0.78
1:B:331:GLU:HG3	4:B:908:HOH:O	1.83	0.78
1:D:684:LYS:HE2	4:D:923:HOH:O	1.81	0.78
1:G:700:THR:HG21	1:G:703:LYS:HB2	1.63	0.78
1:C:339:ASN:CG	4:C:913:HOH:O	2.22	0.78
1:H:661:LYS:HE2	4:H:1609:HOH:O	1.82	0.78
4:G:3308:HOH:O	1:H:714:HIS:HE1	1.67	0.77
1:C:60:ARG:HB3	4:C:2979:HOH:O	1.84	0.75
1:A:799:THR:HG21	4:A:1201:HOH:O	1.85	0.75
1:A:714:HIS:CE1	4:B:3500:HOH:O	2.39	0.75
1:H:11:LYS:HE2	4:H:892:HOH:O	1.86	0.75
1:F:398:GLU:HG3	1:F:406:TRP:CH2	2.22	0.74
1:F:330:THR:HG23	1:F:333:HIS:H	1.51	0.73
1:H:622:GLU:HG3	4:H:3024:HOH:O	1.89	0.73
1:H:398:GLU:HG3	1:H:406:TRP:CZ3	2.24	0.73
1:G:700:THR:HG21	1:G:703:LYS:CB	2.20	0.71
4:G:915:HOH:O	1:H:714:HIS:HB3	1.90	0.71
1:A:714:HIS:HE1	4:B:3500:HOH:O	1.71	0.71
1:A:684:LYS:HE2	4:A:3681:HOH:O	1.89	0.71
4:E:2713:HOH:O	1:F:714:HIS:HD2	1.74	0.71
1:H:398:GLU:HG3	1:H:406:TRP:CH2	2.25	0.71
1:A:62:VAL:HG13	1:B:548:HIS:HA	1.73	0.70
1:H:543:VAL:HG23	1:H:554:GLN:HB3	1.73	0.70
1:C:345:LYS:HD2	4:C:3910:HOH:O	1.92	0.70
1:F:428:ARG:CG	1:F:428:ARG:NH1	2.48	0.70
1:H:335:GLU:HG2	4:H:915:HOH:O	1.92	0.69
1:C:62:VAL:HG13	1:D:548:HIS:HA	1.75	0.69
1:G:468:HIS:HD2	4:G:3974:HOH:O	1.75	0.69
1:F:53:THR:HG23	4:F:910:HOH:O	1.93	0.68
1:E:714:HIS:HB3	4:F:3708:HOH:O	1.92	0.68
1:H:387:LYS:HD2	4:H:4858:HOH:O	1.94	0.68
1:A:144:ALA:HB1	1:A:145:PRO:HD2	1.74	0.68
1:G:353:ASN:CB	4:G:4087:HOH:O	2.32	0.68
4:E:846:HOH:O	1:F:740:THR:HB	1.92	0.68
1:C:366:LYS:HE3	4:C:3467:HOH:O	1.94	0.68
2:B:900:TPP:HN42	2:B:900:TPP:C2	2.07	0.68
1:C:697:ASP:HB2	4:C:3955:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:620:GLU:OE1	1:G:673:ASN:ND2	2.26	0.67
4:C:1489:HOH:O	1:D:714:HIS:HB3	1.93	0.67
1:E:737:GLU:HB3	1:E:749:VAL:CG1	2.24	0.67
1:E:662:LEU:HD13	1:E:758:THR:HG23	1.77	0.67
1:G:170:ASP:OD1	1:G:428:ARG:NH1	2.28	0.67
1:E:737:GLU:CB	1:E:749:VAL:HG12	2.23	0.66
1:C:714:HIS:HE1	4:D:1889:HOH:O	1.78	0.66
1:G:714:HIS:HD2	4:H:2570:HOH:O	1.76	0.66
1:E:741:THR:CG2	1:F:136:PRO:HA	2.23	0.66
1:C:121:LYS:HE3	4:C:1408:HOH:O	1.96	0.66
1:B:121:LYS:HE3	4:B:916:HOH:O	1.96	0.66
1:E:741:THR:HG22	1:F:136:PRO:CA	2.24	0.66
1:F:79:ASN:HD21	1:F:105:GLN:HE21	1.44	0.66
1:E:597:LYS:HE3	4:E:3095:HOH:O	1.97	0.65
1:C:747:VAL:HG22	1:C:752:ILE:HG23	1.79	0.65
1:F:635:LYS:HE2	4:F:2868:HOH:O	1.97	0.64
1:C:11:LYS:HD2	4:C:3667:HOH:O	1.96	0.64
1:E:313:THR:HG21	1:E:323:PRO:HB2	1.79	0.63
1:F:331:GLU:HG2	4:F:3462:HOH:O	1.98	0.63
4:E:4919:HOH:O	1:F:714:HIS:HB3	1.97	0.63
1:A:465:GLU:HG3	4:A:4130:HOH:O	1.99	0.63
1:G:62:VAL:HG13	1:H:548:HIS:HA	1.79	0.63
1:E:740:THR:HG23	4:E:853:HOH:O	1.97	0.63
1:F:144:ALA:HB1	1:F:145:PRO:HD2	1.81	0.63
1:E:398:GLU:HG3	1:E:406:TRP:CH2	2.34	0.63
1:E:665:LEU:HD21	1:E:773:LYS:HD3	1.81	0.63
1:H:714:HIS:CD2	4:H:1694:HOH:O	2.51	0.62
1:H:622:GLU:CG	4:H:3024:HOH:O	2.45	0.62
2:A:900:TPP:HN42	2:A:900:TPP:C2	2.12	0.62
4:C:1489:HOH:O	1:D:714:HIS:CB	2.48	0.62
1:G:530:LYS:HD2	4:G:868:HOH:O	1.98	0.62
1:A:43:ARG:CZ	4:A:921:HOH:O	2.47	0.62
4:E:2490:HOH:O	1:F:714:HIS:CE1	2.39	0.62
1:B:505:VAL:HG11	1:B:558:VAL:HG21	1.82	0.62
1:F:157:LEU:HB3	1:F:184:GLU:HG3	1.82	0.61
1:F:329:ASP:OD1	1:F:330:THR:HG22	2.01	0.61
1:E:20:GLU:HB2	4:E:4923:HOH:O	2.01	0.61
1:F:27:LYS:HB3	1:F:360:VAL:HB	1.82	0.61
1:F:665:LEU:HD21	1:F:773:LYS:HD3	1.83	0.61
1:F:398:GLU:HG3	1:F:406:TRP:CZ3	2.35	0.61
1:A:684:LYS:HD2	4:A:4905:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:THR:HG21	4:D:893:HOH:O	1.99	0.60
1:E:811:LYS:HA	4:E:4837:HOH:O	2.01	0.60
2:C:900:TPP:C2	2:C:900:TPP:HN42	2.15	0.60
4:G:1565:HOH:O	2:H:900:TPP:H2	2.02	0.60
1:F:326:SER:O	1:F:333:HIS:HB3	2.02	0.59
1:C:224:ILE:HG23	1:D:198:LYS:HG3	1.83	0.59
1:C:502:GLU:HG3	1:C:539:VAL:CG1	2.32	0.59
4:A:1803:HOH:O	1:B:714:HIS:HE1	1.84	0.59
1:G:589:GLU:O	1:G:593:LYS:HG3	2.02	0.59
1:E:348:GLU:O	1:E:357:LYS:HE2	2.02	0.59
1:B:170:ASP:OD1	1:B:428:ARG:NH1	2.35	0.59
1:E:498:TRP:CE2	1:E:537:LEU:HD13	2.38	0.58
1:F:597:LYS:HD2	4:F:1505:HOH:O	2.02	0.58
1:E:741:THR:HG21	1:E:745:ASP:OD2	2.03	0.58
1:B:576:TYR:HB3	1:B:587:ILE:HD13	1.84	0.58
1:G:714:HIS:CD2	4:H:2570:HOH:O	2.52	0.57
4:A:849:HOH:O	1:B:714:HIS:CD2	2.57	0.57
1:E:742:THR:HG23	1:F:136:PRO:HG3	1.86	0.57
1:A:322:VAL:O	1:A:322:VAL:HG23	2.04	0.57
1:C:747:VAL:HG13	1:C:753:ASP:HB3	1.85	0.57
1:H:213:HIS:HD2	4:H:931:HOH:O	1.86	0.57
1:B:322:VAL:CG2	1:B:325:ALA:HA	2.34	0.57
1:G:136:PRO:HG3	1:H:742:THR:HG23	1.87	0.57
1:H:498:TRP:CE2	1:H:537:LEU:HD13	2.40	0.57
1:F:597:LYS:HE3	4:F:1505:HOH:O	2.05	0.57
1:C:773:LYS:HG2	4:C:3545:HOH:O	2.05	0.57
1:G:714:HIS:HB3	4:H:1513:HOH:O	2.06	0.56
1:B:640:ALA:O	1:B:703:LYS:HE2	2.04	0.56
1:F:47:LEU:HD12	1:F:123:GLU:HG3	1.86	0.56
1:B:402:TYR:CD1	1:B:813:ALA:HB2	2.40	0.56
1:A:322:VAL:HG13	4:A:906:HOH:O	2.05	0.56
1:B:684:LYS:HE2	4:B:2588:HOH:O	2.04	0.56
1:G:714:HIS:CB	4:H:1513:HOH:O	2.53	0.56
1:G:435:PRO:HA	1:G:476:GLN:O	2.06	0.56
1:E:505:VAL:HG11	1:E:558:VAL:HG21	1.86	0.56
1:H:133:PHE:CD2	1:H:134:SER:HB2	2.41	0.56
1:A:136:PRO:HB3	1:B:741:THR:HG22	1.87	0.56
1:D:739:SER:HB2	4:D:2471:HOH:O	2.06	0.56
1:B:144:ALA:HB1	1:B:145:PRO:HD2	1.88	0.55
1:H:49:LYS:HE3	4:H:885:HOH:O	2.06	0.55
1:B:190:LEU:O	1:B:190:LEU:HD13	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:THR:HG22	1:A:800:ASP:OD1	2.06	0.55
2:C:900:TPP:H2	2:C:900:TPP:HN42	1.72	0.55
1:B:684:LYS:CE	4:B:2588:HOH:O	2.53	0.55
1:A:43:ARG:NE	4:A:921:HOH:O	2.39	0.55
1:E:128:LYS:HE3	4:E:4948:HOH:O	2.05	0.55
1:C:552:SER:HB3	1:D:153:GLU:OE2	2.07	0.54
1:F:398:GLU:HG3	1:F:406:TRP:CZ2	2.43	0.54
1:G:809:ASP:HA	4:G:4464:HOH:O	2.06	0.54
1:B:776:GLU:HB2	4:B:945:HOH:O	2.07	0.54
2:A:900:TPP:HM41	1:B:477:LEU:HD22	1.90	0.54
1:C:326:SER:O	1:C:333:HIS:HB3	2.08	0.54
1:E:545:ARG:HE	1:E:606:GLN:HG3	1.73	0.54
1:E:136:PRO:HG3	1:F:742:THR:HG23	1.89	0.54
1:G:700:THR:HG21	1:G:703:LYS:H	1.71	0.53
1:D:420:ARG:HD2	1:D:421:ASP:OD1	2.08	0.53
1:B:322:VAL:HG21	1:B:325:ALA:HA	1.89	0.53
1:D:90:VAL:HG13	1:D:174:LEU:HD11	1.89	0.53
1:B:61:LEU:HD11	4:B:4128:HOH:O	2.07	0.53
1:C:60:ARG:HD2	4:C:2904:HOH:O	2.07	0.53
1:A:121:LYS:NZ	4:A:860:HOH:O	2.41	0.53
1:A:170:ASP:OD1	1:A:428:ARG:NH1	2.41	0.53
1:D:745:ASP:OD1	1:D:748:ARG:NH2	2.38	0.53
1:A:740:THR:CG2	1:B:140:PRO:HA	2.38	0.53
1:C:811:LYS:HB3	4:C:3127:HOH:O	2.08	0.53
4:A:849:HOH:O	1:B:714:HIS:HD2	1.89	0.53
2:A:900:TPP:H2	4:B:4638:HOH:O	2.08	0.53
1:A:345:LYS:HD2	4:A:3045:HOH:O	2.08	0.53
2:H:900:TPP:HN42	2:H:900:TPP:C2	2.22	0.52
1:C:690:LEU:O	1:C:723:ARG:NH2	2.38	0.52
1:A:387:LYS:HD3	4:A:4232:HOH:O	2.08	0.52
1:B:49:LYS:CE	4:B:935:HOH:O	2.47	0.52
1:G:96:GLY:HA3	1:G:153:GLU:O	2.08	0.52
1:B:144:ALA:HA	1:B:153:GLU:HG3	1.91	0.52
1:A:331:GLU:HG3	4:A:867:HOH:O	2.10	0.52
1:F:313:THR:HG23	1:F:323:PRO:HB3	1.92	0.52
1:B:357:LYS:HE2	4:B:865:HOH:O	2.09	0.52
1:A:498:TRP:CE2	1:A:537:LEU:HD13	2.44	0.52
1:C:198:LYS:HD3	1:C:198:LYS:N	2.25	0.52
1:C:392:GLU:HG3	4:C:4328:HOH:O	2.10	0.52
1:F:34:TYR:CE1	1:F:346:PRO:HG3	2.45	0.52
4:E:2791:HOH:O	2:F:900:TPP:H2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:849:HOH:O	1:D:568:HIS:HB2	2.09	0.51
1:D:142:HIS:CD2	1:D:155:GLY:HA2	2.45	0.51
1:D:197:ASN:OD1	1:D:198:LYS:CE	2.56	0.51
1:A:300:LYS:HE2	1:A:320:HIS:HA	1.92	0.51
1:E:545:ARG:HG3	1:E:606:GLN:HG3	1.93	0.51
1:C:813:ALA:HB3	4:C:5002:HOH:O	2.10	0.51
1:C:668:LYS:NZ	4:C:3386:HOH:O	2.44	0.51
1:F:213:HIS:HD2	4:F:944:HOH:O	1.93	0.51
1:G:134:SER:HA	1:H:740:THR:CG2	2.40	0.51
2:B:900:TPP:H2	2:B:900:TPP:HN42	1.75	0.51
1:F:505:VAL:HG11	1:F:558:VAL:HG21	1.92	0.51
1:A:597:LYS:HE2	4:A:2010:HOH:O	2.11	0.51
1:B:322:VAL:HG23	1:B:322:VAL:O	2.09	0.51
1:G:60:ARG:NH1	4:G:843:HOH:O	2.44	0.51
1:H:111:THR:HG21	1:H:372:GLY:C	2.31	0.51
1:F:572:VAL:O	1:F:597:LYS:HA	2.10	0.51
1:G:366:LYS:HG3	4:G:3106:HOH:O	2.11	0.51
1:F:121:LYS:HE2	4:F:2071:HOH:O	2.11	0.51
1:C:655:ILE:HG12	1:C:757:LEU:HD13	1.93	0.51
1:C:144:ALA:HB1	1:C:145:PRO:HD2	1.92	0.50
1:E:313:THR:HG21	1:E:323:PRO:CB	2.40	0.50
4:E:2713:HOH:O	1:F:714:HIS:CD2	2.56	0.50
1:G:646:ALA:HB2	1:G:655:ILE:HG13	1.92	0.50
1:F:398:GLU:CG	1:F:406:TRP:CZ3	2.95	0.50
2:A:900:TPP:H2	2:A:900:TPP:HN42	1.75	0.50
1:H:693:GLU:O	1:H:697:ASP:HB2	2.12	0.50
1:D:545:ARG:HG3	1:D:606:GLN:HG3	1.94	0.50
1:D:576:TYR:HB3	1:D:587:ILE:HD13	1.94	0.50
1:C:338:LYS:HE3	4:C:924:HOH:O	2.11	0.50
1:D:670:LYS:HG3	4:D:4914:HOH:O	2.11	0.49
1:C:118:LYS:HB2	4:C:2404:HOH:O	2.11	0.49
1:C:134:SER:HB2	1:D:740:THR:HG21	1.92	0.49
1:G:700:THR:HG22	1:G:703:LYS:H	1.69	0.49
1:A:13:LEU:HD23	4:A:4379:HOH:O	2.12	0.49
1:E:410:GLU:HG2	1:E:605:LYS:O	2.12	0.49
1:F:709:TYR:CE2	1:F:711:SER:HB3	2.47	0.49
1:B:632:SER:HB3	1:B:670:LYS:HA	1.93	0.49
1:F:14:ASN:HB3	4:F:921:HOH:O	2.11	0.49
1:D:568:HIS:HE1	4:D:914:HOH:O	1.95	0.49
1:G:477:LEU:HD22	2:H:900:TPP:HM41	1.94	0.49
1:A:740:THR:HG21	1:B:140:PRO:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:463:VAL:HG21	1:H:217:TYR:OH	2.12	0.49
1:E:428:ARG:HH11	1:E:428:ARG:HG3	1.77	0.49
1:E:366:LYS:HE2	4:E:917:HOH:O	2.12	0.49
1:G:714:HIS:CE1	4:H:935:HOH:O	2.66	0.49
4:A:1803:HOH:O	1:B:714:HIS:CE1	2.60	0.49
2:F:900:TPP:HN42	2:F:900:TPP:C2	2.25	0.49
1:A:338:LYS:NZ	4:A:937:HOH:O	2.44	0.49
1:B:120:THR:O	1:B:125:GLY:HA3	2.13	0.49
1:F:583:MET:HA	1:F:617:ALA:HB1	1.95	0.48
1:A:796:PRO:O	1:A:800:ASP:HB2	2.13	0.48
1:B:304:CYS:HB2	1:B:305:PRO:CD	2.43	0.48
4:A:3876:HOH:O	1:H:779:LYS:HE3	2.13	0.48
1:E:398:GLU:HG3	1:E:406:TRP:CZ2	2.47	0.48
1:G:740:THR:HG21	1:H:134:SER:OG	2.13	0.48
1:C:139:ILE:HB	1:C:140:PRO:CD	2.43	0.48
1:H:326:SER:O	1:H:333:HIS:HB3	2.14	0.48
1:D:121:LYS:HE3	4:D:1097:HOH:O	2.12	0.48
1:E:420:ARG:HD2	1:E:421:ASP:OD1	2.13	0.48
1:H:546:GLN:OE1	1:H:549:ASN:HB2	2.14	0.48
1:C:747:VAL:HG13	1:C:753:ASP:CB	2.42	0.48
1:A:313:THR:CG2	1:A:323:PRO:HB3	2.44	0.48
4:G:3308:HOH:O	1:H:714:HIS:CE1	2.52	0.48
1:E:2:THR:N	4:E:4555:HOH:O	2.47	0.48
1:H:252:ASP:HB2	4:H:3323:HOH:O	2.13	0.48
1:D:540:SER:O	1:D:541:SER:C	2.52	0.48
1:A:435:PRO:HA	1:A:476:GLN:O	2.14	0.47
1:G:454:TRP:CZ2	1:G:456:ALA:HB3	2.49	0.47
1:F:345:LYS:HE3	4:F:919:HOH:O	2.14	0.47
1:G:714:HIS:HE1	4:H:935:HOH:O	1.97	0.47
1:E:215:ASN:HA	1:E:298:THR:O	2.14	0.47
1:F:646:ALA:HB2	1:F:655:ILE:HG13	1.95	0.47
1:H:60:ARG:CD	4:H:880:HOH:O	2.47	0.47
2:E:900:TPP:C2	2:E:900:TPP:HN42	2.27	0.47
1:E:144:ALA:HB1	1:E:145:PRO:HD2	1.96	0.47
1:C:807:ASN:ND2	1:C:810:LYS:HG3	2.30	0.47
1:C:468:HIS:CD2	4:C:2876:HOH:O	2.68	0.47
1:F:49:LYS:HD2	4:F:911:HOH:O	2.15	0.47
1:H:144:ALA:HB1	1:H:145:PRO:HD2	1.95	0.47
1:E:387:LYS:HE2	4:E:3017:HOH:O	2.14	0.47
1:E:94:GLY:N	1:E:95:PRO:CD	2.77	0.47
1:H:33:ASN:O	1:H:37:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PRO:HB2	1:D:10:TRP:CD1	2.50	0.47
1:E:313:THR:CG2	1:E:323:PRO:HB3	2.45	0.47
1:C:697:ASP:CB	4:C:3955:HOH:O	2.56	0.47
1:E:741:THR:HB	1:E:742:THR:H	1.37	0.47
1:G:134:SER:HA	1:H:740:THR:HG21	1.97	0.47
1:F:540:SER:O	1:F:541:SER:C	2.53	0.46
1:C:227:ARG:HD2	1:D:457:GLY:O	2.15	0.46
1:A:215:ASN:HA	1:A:298:THR:O	2.14	0.46
1:C:60:ARG:CD	4:C:2904:HOH:O	2.61	0.46
1:H:161:LEU:HD23	1:H:161:LEU:HA	1.71	0.46
1:B:325:ALA:HB2	4:B:4983:HOH:O	2.15	0.46
1:D:323:PRO:O	1:D:324:LEU:HB2	2.15	0.46
1:F:545:ARG:HA	1:F:545:ARG:HD2	1.75	0.46
1:F:330:THR:HG21	4:F:3116:HOH:O	2.16	0.46
1:E:477:LEU:HD22	2:F:900:TPP:HM41	1.98	0.46
1:F:35:LEU:O	1:F:39:GLN:HG3	2.16	0.46
2:D:900:TPP:HN42	2:D:900:TPP:C2	2.29	0.46
1:B:231:GLU:H	1:B:231:GLU:CD	2.18	0.46
1:G:366:LYS:HG3	4:G:2856:HOH:O	2.15	0.46
1:F:737:GLU:HB3	1:F:749:VAL:HG13	1.96	0.46
1:H:612:LEU:HD21	1:H:628:TRP:CE2	2.51	0.46
1:H:630:TRP:CZ3	1:H:631:ALA:HB2	2.50	0.46
1:G:313:THR:HG21	1:G:323:PRO:HB2	1.98	0.46
1:D:489:TYR:CE2	1:D:494:ARG:HB3	2.51	0.46
1:D:620:GLU:OE1	1:D:673:ASN:ND2	2.45	0.46
2:E:900:TPP:HM41	1:F:477:LEU:HD22	1.98	0.46
1:B:142:HIS:CD2	1:B:155:GLY:HA2	2.51	0.46
1:E:68:THR:N	1:E:69:PRO:HD2	2.31	0.46
1:F:165:TYR:CD2	1:F:196:SER:HB2	2.51	0.46
1:G:390:ASN:CB	4:G:3444:HOH:O	2.34	0.45
1:E:313:THR:CG2	1:E:323:PRO:CB	2.94	0.45
1:A:430:PHE:HA	1:A:495:HIS:O	2.16	0.45
1:A:190:LEU:HD13	1:A:190:LEU:O	2.16	0.45
1:D:589:GLU:OE1	4:D:933:HOH:O	2.21	0.45
1:H:714:HIS:HD2	4:H:1694:HOH:O	1.96	0.45
1:F:435:PRO:HA	1:F:476:GLN:O	2.15	0.45
1:F:483:GLU:OE1	1:F:487:GLU:OE1	2.34	0.45
1:H:50:GLU:HG2	4:H:883:HOH:O	2.15	0.45
1:B:681:GLN:O	1:B:723:ARG:NH2	2.48	0.45
1:E:151:ILE:CG2	1:E:377:ALA:HA	2.46	0.45
1:D:737:GLU:HB3	1:D:749:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:TYR:CD1	1:G:136:PRO:HD2	2.51	0.45
1:E:428:ARG:HG3	1:E:428:ARG:NH1	2.31	0.45
1:B:304:CYS:HB2	1:B:305:PRO:HD2	1.99	0.45
1:B:351:ASP:OD1	1:B:351:ASP:C	2.55	0.45
1:B:430:PHE:HA	1:B:495:HIS:O	2.17	0.45
1:D:478:SER:HB3	1:D:481:GLN:HB2	1.97	0.45
1:D:420:ARG:CD	1:D:421:ASP:OD1	2.65	0.45
1:H:108:LEU:HD22	1:H:361:LEU:HD21	1.99	0.45
1:A:28:TYR:C	1:A:28:TYR:CD2	2.90	0.45
2:G:900:TPP:C2	2:G:900:TPP:HN42	2.29	0.45
1:C:468:HIS:HD2	4:C:2876:HOH:O	1.99	0.45
1:E:218:LYS:HB2	1:F:436:ASP:OD2	2.16	0.45
1:E:775:ASP:O	1:E:779:LYS:HG2	2.16	0.45
1:A:134:SER:HB3	1:B:740:THR:HG21	1.99	0.45
1:F:811:LYS:HD3	1:F:811:LYS:HA	1.63	0.45
1:G:301:GLY:O	1:G:302:TRP:C	2.55	0.45
1:H:661:LYS:O	1:H:664:GLU:HG2	2.17	0.45
1:C:589:GLU:HG2	1:C:593:LYS:HD2	1.99	0.45
1:G:490:LEU:HD11	1:G:535:MET:HA	1.99	0.45
1:A:773:LYS:HG2	4:A:875:HOH:O	2.16	0.45
1:C:10:TRP:CD2	1:C:278:LYS:HG3	2.52	0.45
1:H:215:ASN:HA	1:H:298:THR:O	2.16	0.45
1:D:661:LYS:NZ	4:D:899:HOH:O	2.49	0.45
1:D:498:TRP:CE2	1:D:537:LEU:HD13	2.52	0.45
1:A:288:ARG:HD3	1:A:455:ASP:O	2.17	0.44
1:E:772:ASP:HB2	4:E:2793:HOH:O	2.16	0.44
1:H:345:LYS:N	1:H:346:PRO:CD	2.80	0.44
1:G:540:SER:O	1:G:541:SER:C	2.56	0.44
1:D:630:TRP:CZ3	1:D:631:ALA:HB2	2.51	0.44
1:H:80:ARG:C	1:H:80:ARG:HD2	2.38	0.44
1:G:546:GLN:O	4:G:927:HOH:O	2.21	0.44
1:H:10:TRP:CZ2	1:H:278:LYS:HE3	2.52	0.44
1:C:38:GLY:HA3	1:C:130:PHE:CE2	2.53	0.44
1:C:65:TRP:HE1	1:C:304:CYS:HB3	1.83	0.44
1:B:65:TRP:HB3	1:B:323:PRO:HD3	2.00	0.44
1:C:300:LYS:HE2	1:C:320:HIS:HA	1.99	0.44
1:D:702:ASP:OD1	1:D:702:ASP:N	2.51	0.44
1:A:668:LYS:HD3	1:A:668:LYS:HA	1.65	0.44
1:C:168:ILE:HD13	1:C:208:VAL:HG23	1.98	0.44
1:C:714:HIS:HD2	4:D:867:HOH:O	2.01	0.44
1:A:331:GLU:HG2	4:A:854:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:699:PHE:O	1:G:700:THR:CB	2.44	0.44
1:G:479:GLU:OE2	2:H:900:TPP:N1'	2.50	0.44
1:H:520:GLU:O	1:H:524:ARG:HG3	2.17	0.44
1:D:300:LYS:HE2	1:D:320:HIS:HA	2.00	0.44
1:H:274:ILE:HG13	1:H:292:PRO:HG2	2.00	0.44
1:B:300:LYS:HG2	1:B:319:SER:OG	2.17	0.44
1:C:121:LYS:CE	4:C:1408:HOH:O	2.60	0.44
1:E:151:ILE:HG23	1:E:377:ALA:HA	1.99	0.44
1:F:636:ASN:ND2	1:F:639:GLU:H	2.15	0.44
1:A:639:GLU:HG2	1:A:639:GLU:O	2.18	0.44
1:F:520:GLU:O	1:F:524:ARG:HG3	2.17	0.44
1:E:366:LYS:NZ	4:E:917:HOH:O	2.50	0.44
2:D:900:TPP:HN42	2:D:900:TPP:H2	1.83	0.44
1:E:661:LYS:HE3	4:E:925:HOH:O	2.18	0.43
1:G:190:LEU:HD13	1:G:190:LEU:O	2.18	0.43
1:E:436:ASP:OD1	1:F:218:LYS:HB2	2.18	0.43
1:C:180:VAL:HG11	1:C:190:LEU:HD11	1.99	0.43
1:C:11:LYS:HE2	4:C:3667:HOH:O	2.18	0.43
1:F:238:HIS:HA	1:F:242:TYR:O	2.18	0.43
1:B:435:PRO:HA	1:B:476:GLN:O	2.18	0.43
1:A:548:HIS:HA	1:B:62:VAL:HG13	2.00	0.43
1:H:391:LEU:HD12	1:H:391:LEU:HA	1.86	0.43
1:G:787:PHE:CD2	1:G:787:PHE:C	2.90	0.43
1:E:398:GLU:HG3	1:E:406:TRP:CZ3	2.53	0.43
1:B:96:GLY:HA3	1:B:153:GLU:O	2.18	0.43
1:A:739:SER:HB2	1:A:740:THR:H	1.60	0.43
1:H:306:LYS:HG3	4:H:2443:HOH:O	2.17	0.43
1:G:700:THR:HG23	1:G:702:ASP:H	1.83	0.43
1:E:545:ARG:NE	1:E:606:GLN:HG3	2.33	0.43
1:B:94:GLY:N	1:B:95:PRO:CD	2.82	0.43
1:B:583:MET:HA	1:B:617:ALA:HB1	2.00	0.43
1:F:50:GLU:HA	1:F:51:PRO:HA	1.83	0.43
1:D:748:ARG:HA	1:D:753:ASP:OD2	2.19	0.43
1:D:120:THR:O	1:D:125:GLY:HA3	2.18	0.43
1:E:190:LEU:HD13	1:E:190:LEU:O	2.19	0.43
1:A:198:LYS:HG3	1:B:224:ILE:HG23	2.01	0.43
1:D:392:GLU:OE2	1:D:618:ARG:NH2	2.51	0.43
4:C:1868:HOH:O	1:D:714:HIS:CE1	2.72	0.43
1:F:435:PRO:O	1:F:436:ASP:HB3	2.19	0.43
1:G:442:ARG:HG2	4:G:3978:HOH:O	2.18	0.43
1:C:34:TYR:CE1	1:C:341:LEU:HD22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:GLY:HA3	4:D:2297:HOH:O	2.19	0.43
1:D:152:HIS:HB3	4:D:948:HOH:O	2.18	0.42
1:G:620:GLU:CD	1:G:673:ASN:HD22	2.17	0.42
1:C:714:HIS:CE1	4:D:1889:HOH:O	2.62	0.42
1:B:322:VAL:HG23	1:B:325:ALA:HA	2.02	0.42
1:D:647:ALA:HB2	1:D:674:VAL:HB	2.00	0.42
1:F:51:PRO:HD2	4:F:3885:HOH:O	2.19	0.42
1:B:190:LEU:C	1:B:190:LEU:HD13	2.39	0.42
1:E:36:SER:O	1:E:40:ILE:HG13	2.20	0.42
1:A:477:LEU:HD22	2:B:900:TPP:HM41	2.00	0.42
1:H:238:HIS:HA	1:H:242:TYR:O	2.20	0.42
1:C:505:VAL:HG11	1:C:558:VAL:HG21	2.01	0.42
1:F:10:TRP:CZ2	1:F:278:LYS:HE3	2.55	0.42
1:E:31:VAL:O	1:E:35:LEU:HG	2.20	0.42
1:G:135:TYR:CG	1:G:136:PRO:HD2	2.54	0.42
1:G:218:LYS:HB2	1:H:436:ASP:OD2	2.19	0.42
1:B:230:ASP:OD2	1:B:246:GLU:OE1	2.37	0.42
1:E:391:LEU:HD23	1:E:614:LEU:HD11	2.02	0.42
1:H:257:MET:O	1:H:261:ARG:HG3	2.20	0.42
1:C:583:MET:HA	1:C:617:ALA:HB1	2.02	0.42
1:G:436:ASP:OD2	1:H:218:LYS:HB2	2.19	0.42
1:B:215:ASN:HA	1:B:298:THR:O	2.20	0.42
1:F:330:THR:CG2	1:F:333:HIS:ND1	2.83	0.42
1:C:744:TYR:O	1:C:747:VAL:HG12	2.19	0.42
1:H:630:TRP:CE3	1:H:631:ALA:HB2	2.55	0.42
1:B:330:THR:HB	4:B:928:HOH:O	2.20	0.42
1:E:414:THR:HG23	4:E:3125:HOH:O	2.19	0.42
1:B:213:HIS:HD2	4:B:960:HOH:O	2.02	0.42
1:G:700:THR:CG2	1:G:702:ASP:H	2.33	0.42
1:F:737:GLU:CB	1:F:749:VAL:HG13	2.49	0.42
1:G:313:THR:CG2	1:G:323:PRO:HB3	2.50	0.42
1:C:20:GLU:HB2	4:C:3097:HOH:O	2.20	0.42
1:D:435:PRO:HA	1:D:476:GLN:O	2.20	0.42
1:F:360:VAL:HG22	1:F:361:LEU:HG	2.01	0.42
1:C:759:ALA:O	1:C:763:ARG:HG3	2.19	0.42
1:A:583:MET:HA	1:A:617:ALA:HB1	2.01	0.42
1:C:486:LEU:O	1:C:490:LEU:HG	2.20	0.41
1:B:646:ALA:HB2	1:B:655:ILE:HG13	2.02	0.41
1:C:758:THR:HG22	1:C:777:LEU:HD21	2.01	0.41
1:A:657:ALA:HA	1:A:801:TRP:CZ2	2.55	0.41
1:B:636:ASN:HD22	1:B:638:ASP:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:630:TRP:CZ3	1:C:631:ALA:HB2	2.56	0.41
1:F:424:LYS:HG2	1:F:424:LYS:O	2.20	0.41
1:G:799:THR:HB	4:G:1461:HOH:O	2.19	0.41
1:C:552:SER:HB3	4:D:3699:HOH:O	2.19	0.41
1:A:170:ASP:HA	1:A:428:ARG:NH1	2.35	0.41
1:C:755:TYR:CZ	1:C:780:PHE:HE2	2.38	0.41
1:G:261:ARG:HD2	4:G:2429:HOH:O	2.20	0.41
1:F:545:ARG:HG3	1:F:606:GLN:HG3	2.03	0.41
1:F:498:TRP:CE2	1:F:537:LEU:HD13	2.55	0.41
1:G:700:THR:CG2	1:G:703:LYS:N	2.64	0.41
1:A:740:THR:HG23	4:A:4838:HOH:O	2.20	0.41
2:E:900:TPP:H2	4:F:3773:HOH:O	2.21	0.41
1:D:811:LYS:HB2	4:D:3140:HOH:O	2.20	0.41
1:G:188:GLY:HA2	1:H:192:THR:HB	2.01	0.41
1:F:53:THR:CG2	4:F:910:HOH:O	2.61	0.41
1:E:213:HIS:HD2	4:E:947:HOH:O	2.03	0.41
1:C:50:GLU:HA	1:C:51:PRO:HA	1.76	0.41
1:H:622:GLU:HG2	4:H:3024:HOH:O	2.19	0.41
1:A:170:ASP:HA	1:A:428:ARG:HH12	1.86	0.41
1:F:31:VAL:O	1:F:35:LEU:HG	2.20	0.41
1:A:27:LYS:HB3	1:A:360:VAL:HG13	2.01	0.41
1:H:181:GLY:HA3	4:H:889:HOH:O	2.20	0.41
2:H:900:TPP:H2	2:H:900:TPP:HN42	1.85	0.41
1:H:213:HIS:CD2	4:H:931:HOH:O	2.69	0.41
1:F:126:LEU:HD11	1:F:350:PHE:CE1	2.56	0.41
1:D:261:ARG:NH2	4:D:2506:HOH:O	2.50	0.41
1:F:215:ASN:HA	1:F:298:THR:O	2.21	0.41
1:D:369:LEU:HA	1:D:369:LEU:HD23	1.92	0.41
1:C:414:THR:HG22	1:C:585:LEU:HD21	2.03	0.41
1:G:583:MET:HA	1:G:617:ALA:HB1	2.02	0.41
1:A:442:ARG:HA	1:A:444:GLN:OE1	2.21	0.41
1:A:383:ARG:NH1	4:A:4116:HOH:O	2.51	0.41
1:A:65:TRP:O	1:A:69:PRO:HD2	2.21	0.41
1:F:300:LYS:HG2	1:F:319:SER:OG	2.20	0.41
1:A:68:THR:N	1:A:69:PRO:HD2	2.35	0.41
1:A:379:GLY:HA3	1:A:491:LEU:O	2.21	0.41
1:H:180:VAL:HG11	1:H:190:LEU:HD11	2.03	0.41
1:C:65:TRP:NE1	1:C:304:CYS:HB3	2.36	0.40
1:C:442:ARG:HE	1:C:605:LYS:HB2	1.86	0.40
1:G:744:TYR:OH	1:G:781:ARG:HA	2.21	0.40
1:H:126:LEU:HD11	1:H:350:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:GLU:HB3	1:C:605:LYS:O	2.21	0.40
1:D:755:TYR:CZ	1:D:780:PHE:HE2	2.39	0.40
1:G:647:ALA:HB2	1:G:674:VAL:HB	2.02	0.40
1:G:717:ARG:HD3	1:H:721:TYR:CG	2.56	0.40
1:H:597:LYS:HB3	1:H:597:LYS:HE3	1.79	0.40
1:G:468:HIS:CD2	4:G:3974:HOH:O	2.59	0.40
1:E:134:SER:HA	1:F:740:THR:HG21	2.03	0.40
1:C:744:TYR:HB3	1:C:794:ASP:CG	2.42	0.40
1:D:490:LEU:HD21	1:D:535:MET:HA	2.04	0.40
1:C:17:VAL:HG21	1:C:264:ALA:HB1	2.03	0.40
1:F:704:PRO:HA	1:F:728:ASN:HB3	2.03	0.40
1:F:28:TYR:CD2	1:F:28:TYR:C	2.95	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:871:HOH:O	4:E:941:HOH:O[1_656]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	811/831 (98%)	776 (96%)	34 (4%)	1 (0%)	56	64
1	B	811/831 (98%)	773 (95%)	37 (5%)	1 (0%)	56	64
1	C	811/831 (98%)	769 (95%)	41 (5%)	1 (0%)	56	64
1	D	811/831 (98%)	770 (95%)	40 (5%)	1 (0%)	56	64
1	E	811/831 (98%)	769 (95%)	39 (5%)	3 (0%)	39	42
1	F	811/831 (98%)	768 (95%)	42 (5%)	1 (0%)	56	64
1	G	811/831 (98%)	769 (95%)	40 (5%)	2 (0%)	52	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	811/831 (98%)	777 (96%)	32 (4%)	2 (0%)	52	59
All	All	6488/6648 (98%)	6171 (95%)	305 (5%)	12 (0%)	52	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	811	LYS
1	B	811	LYS
1	F	302	TRP
1	A	302	TRP
1	C	739	SER
1	D	714	HIS
1	G	700	THR
1	G	702	ASP
1	H	302	TRP
1	E	303	THR
1	E	754	ARG
1	H	739	SER

### 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	680/693 (98%)	666 (98%)	14 (2%)	61	74
1	B	680/693 (98%)	661 (97%)	19 (3%)	51	63
1	C	680/693 (98%)	662 (97%)	18 (3%)	54	66
1	D	680/693 (98%)	654 (96%)	26 (4%)	40	49
1	E	680/693 (98%)	668 (98%)	12 (2%)	66	79
1	F	680/693 (98%)	660 (97%)	20 (3%)	50	62
1	G	680/693 (98%)	662 (97%)	18 (3%)	54	66
1	H	680/693 (98%)	666 (98%)	14 (2%)	61	74
All	All	5440/5544 (98%)	5299 (97%)	141 (3%)	54	66

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	105	GLN
1	A	147	THR
1	A	198	LYS
1	A	366	LYS
1	A	369	LEU
1	A	429	ASP
1	A	477	LEU
1	A	494	ARG
1	A	684	LYS
1	A	740	THR
1	A	777	LEU
1	A	810	LYS
1	A	811	LYS
1	B	20	GLU
1	B	35	LEU
1	B	105	GLN
1	B	147	THR
1	B	321	GLN
1	B	326	SER
1	B	330	THR
1	B	356	VAL
1	B	386	LEU
1	B	387	LYS
1	B	388	LEU
1	B	477	LEU
1	B	563	LEU
1	B	623	LYS
1	B	636	ASN
1	B	719	LEU
1	B	741	THR
1	B	773	LYS
1	B	814	VAL
1	C	35	LEU
1	C	105	GLN
1	C	134	SER
1	C	190	LEU
1	C	198	LYS
1	C	213	HIS
1	C	335	GLU
1	C	429	ASP
1	C	442	ARG

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Mol	Chain	Res	Type
1	C	477	LEU
1	C	494	ARG
1	C	597	LYS
1	C	623	LYS
1	C	690	LEU
1	C	693	GLU
1	C	740	THR
1	C	747	VAL
1	C	777	LEU
1	D	50	GLU
1	D	105	GLN
1	D	146	GLU
1	D	147	THR
1	D	198	LYS
1	D	266	LEU
1	D	321	GLN
1	D	341	LEU
1	D	390	ASN
1	D	424	LYS
1	D	429	ASP
1	D	449	VAL
1	D	477	LEU
1	D	490	LEU
1	D	494	ARG
1	D	622	GLU
1	D	635	LYS
1	D	659	SER
1	D	664	GLU
1	D	693	GLU
1	D	749	VAL
1	D	775	ASP
1	D	802	VAL
1	D	808	THR
1	D	810	LYS
1	D	814	VAL
1	E	105	GLN
1	E	147	THR
1	E	311	LYS
1	E	429	ASP
1	E	446	SER
1	E	477	LEU
1	E	662	LEU

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Mol	Chain	Res	Type
1	E	739	SER
1	E	740	THR
1	E	741	THR
1	E	773	LYS
1	E	776	GLU
1	F	50	GLU
1	F	53	THR
1	F	134	SER
1	F	299	PRO
1	F	306	LYS
1	F	313	THR
1	F	390	ASN
1	F	428	ARG
1	F	429	ASP
1	F	446	SER
1	F	449	VAL
1	F	477	LEU
1	F	605	LYS
1	F	618	ARG
1	F	636	ASN
1	F	639	GLU
1	F	697	ASP
1	F	749	VAL
1	F	775	ASP
1	F	811	LYS
1	G	44	SER
1	G	60	ARG
1	G	105	GLN
1	G	147	THR
1	G	231	GLU
1	G	258	SER
1	G	266	LEU
1	G	331	GLU
1	G	424	LYS
1	G	429	ASP
1	G	467	MET
1	G	477	LEU
1	G	560	SER
1	G	563	LEU
1	G	635	LYS
1	G	684	LYS
1	G	700	THR

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Mol	Chain	Res	Type
1	G	707	PHE
1	H	20	GLU
1	H	55	GLU
1	H	100	PRO
1	H	105	GLN
1	H	134	SER
1	H	147	THR
1	H	190	LEU
1	H	306	LYS
1	H	341	LEU
1	H	383	ARG
1	H	519	LEU
1	H	622	GLU
1	H	775	ASP
1	H	796	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	HIS
1	A	653	GLN
1	A	714	HIS
1	B	213	HIS
1	B	568	HIS
1	B	636	ASN
1	B	714	HIS
1	C	714	HIS
1	D	714	HIS
1	E	213	HIS
1	E	714	HIS
1	F	105	GLN
1	F	213	HIS
1	F	636	ASN
1	F	714	HIS
1	G	653	GLN
1	G	714	HIS
1	H	213	HIS
1	H	714	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
2	TPP	A	900	3	20,27,27	2.14	4 (20%)	31,40,40	2.24	10 (32%)
2	TPP	B	900	3	20,27,27	2.27	4 (20%)	31,40,40	2.42	14 (45%)
2	TPP	C	900	3	20,27,27	2.11	5 (25%)	31,40,40	2.13	11 (35%)
2	TPP	D	900	3	20,27,27	1.95	4 (20%)	31,40,40	2.32	12 (38%)
2	TPP	E	900	3	20,27,27	2.07	4 (20%)	31,40,40	2.04	8 (25%)
2	TPP	F	900	3	20,27,27	1.98	4 (20%)	31,40,40	2.00	7 (22%)
2	TPP	G	900	3	20,27,27	2.08	3 (15%)	31,40,40	2.48	12 (38%)
2	TPP	H	900	3	20,27,27	2.15	3 (15%)	31,40,40	2.43	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	900	3	-	0/16/17/17	0/2/2/2
2	TPP	B	900	3	-	0/16/17/17	0/2/2/2
2	TPP	C	900	3	-	0/16/17/17	0/2/2/2
2	TPP	D	900	3	-	0/16/17/17	0/2/2/2
2	TPP	E	900	3	-	0/16/17/17	0/2/2/2
2	TPP	F	900	3	-	0/16/17/17	0/2/2/2
2	TPP	G	900	3	-	0/16/17/17	0/2/2/2
2	TPP	H	900	3	-	0/16/17/17	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	TPP	C4-N3	-3.31	1.36	1.39
2	E	900	TPP	C4-N3	-3.13	1.37	1.39
2	A	900	TPP	C4-N3	-2.18	1.37	1.39
2	F	900	TPP	C4'-N3'	2.11	1.38	1.35
2	C	900	TPP	C4'-N3'	2.21	1.38	1.35
2	C	900	TPP	CM4-C4	2.26	1.54	1.49
2	D	900	TPP	PB-O1B	2.98	1.61	1.51
2	F	900	TPP	PA-O2A	3.20	1.68	1.54
2	G	900	TPP	PA-O2A	3.23	1.68	1.54
2	A	900	TPP	PA-O2A	3.64	1.70	1.54
2	D	900	TPP	PB-O3B	3.65	1.67	1.54
2	B	900	TPP	PA-O2A	4.04	1.72	1.54
2	E	900	TPP	PA-O2A	4.24	1.73	1.54
2	H	900	TPP	PA-O2A	4.34	1.73	1.54
2	D	900	TPP	PA-O2A	4.37	1.73	1.54
2	C	900	TPP	PA-O2A	4.38	1.73	1.54
2	C	900	TPP	PB-O2B	4.50	1.70	1.54
2	D	900	TPP	PB-O2B	4.52	1.71	1.54
2	A	900	TPP	PB-O3B	4.58	1.71	1.54
2	E	900	TPP	PB-O2B	4.61	1.71	1.54
2	E	900	TPP	PB-O3B	4.71	1.71	1.54
2	H	900	TPP	PB-O3B	4.79	1.71	1.54
2	F	900	TPP	PB-O3B	4.96	1.72	1.54
2	C	900	TPP	PB-O3B	5.11	1.73	1.54
2	F	900	TPP	PB-O2B	5.14	1.73	1.54
2	B	900	TPP	PB-O3B	5.33	1.73	1.54
2	H	900	TPP	PB-O2B	5.40	1.74	1.54
2	G	900	TPP	PB-O2B	5.47	1.74	1.54
2	B	900	TPP	PB-O2B	5.50	1.74	1.54
2	G	900	TPP	PB-O3B	5.53	1.74	1.54
2	A	900	TPP	PB-O2B	5.64	1.75	1.54

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	900	TPP	C6-C5-S1	-5.36	112.74	120.24
2	B	900	TPP	N1'-C2'-N3'	-4.00	118.21	125.60
2	F	900	TPP	N1'-C2'-N3'	-3.88	118.42	125.60
2	D	900	TPP	CM4-C4-C5	-3.88	120.18	128.90
2	G	900	TPP	C6-C5-S1	-3.75	114.99	120.24
2	D	900	TPP	C5'-C6'-N1'	-3.59	117.62	123.86
2	B	900	TPP	C5'-C4'-N4'	-3.59	116.99	122.25
2	A	900	TPP	N1'-C2'-N3'	-3.58	118.97	125.60
2	A	900	TPP	C5'-C7'-N3	-3.56	107.37	113.33
2	E	900	TPP	CM4-C4-C5	-3.45	121.14	128.90
2	C	900	TPP	CM4-C4-C5	-3.31	121.47	128.90
2	B	900	TPP	CM4-C4-C5	-3.23	121.65	128.90
2	B	900	TPP	C5'-C6'-N1'	-3.20	118.30	123.86
2	F	900	TPP	CM4-C4-C5	-3.17	121.77	128.90
2	G	900	TPP	CM4-C4-C5	-3.13	121.85	128.90
2	G	900	TPP	N1'-C2'-N3'	-3.13	119.80	125.60
2	H	900	TPP	N1'-C2'-N3'	-3.09	119.89	125.60
2	A	900	TPP	CM4-C4-C5	-3.08	121.97	128.90
2	C	900	TPP	N1'-C2'-N3'	-3.05	119.95	125.60
2	G	900	TPP	C5'-C7'-N3	-3.02	108.28	113.33
2	D	900	TPP	C6-C5-S1	-2.95	116.11	120.24
2	E	900	TPP	N1'-C2'-N3'	-2.94	120.16	125.60
2	G	900	TPP	C5'-C6'-N1'	-2.92	118.79	123.86
2	B	900	TPP	C6-C5-S1	-2.73	116.42	120.24
2	C	900	TPP	C5'-C6'-N1'	-2.66	119.23	123.86
2	B	900	TPP	PA-O3A-PB	-2.58	124.01	132.67
2	C	900	TPP	C6-C5-S1	-2.55	116.68	120.24
2	A	900	TPP	C6-C5-S1	-2.42	116.85	120.24
2	D	900	TPP	C7'-C5'-C6'	-2.40	115.75	120.67
2	F	900	TPP	C6-C5-S1	-2.31	117.01	120.24
2	A	900	TPP	PA-O3A-PB	-2.29	124.99	132.67
2	H	900	TPP	PA-O3A-PB	-2.23	125.18	132.67
2	E	900	TPP	O7-PA-O1A	-2.18	101.17	109.62
2	C	900	TPP	PA-O3A-PB	-2.17	125.39	132.67
2	H	900	TPP	CM4-C4-C5	-2.14	124.09	128.90
2	E	900	TPP	C6-C5-S1	-2.12	117.28	120.24
2	D	900	TPP	N1'-C2'-N3'	-2.09	121.73	125.60
2	B	900	TPP	O7-PA-O1A	-2.09	101.52	109.62
2	B	900	TPP	C5'-C7'-N3	-2.04	109.91	113.33
2	D	900	TPP	C5'-C4'-N3'	-2.02	117.86	121.23
2	G	900	TPP	C7'-C5'-C6'	-2.01	116.56	120.67
2	E	900	TPP	C5'-C4'-N3'	-2.00	117.89	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	TPP	CM2-C2'-N1'	2.04	119.48	117.03
2	A	900	TPP	CM2-C2'-N3'	2.12	120.81	117.20
2	G	900	TPP	C5-C4-N3	2.14	112.40	107.69
2	C	900	TPP	O2B-PB-O3A	2.16	114.88	105.09
2	H	900	TPP	C5-C4-N3	2.18	112.49	107.69
2	D	900	TPP	CM4-C4-N3	2.34	125.71	122.59
2	H	900	TPP	CM2-C2'-N1'	2.35	119.84	117.03
2	G	900	TPP	CM4-C4-N3	2.37	125.75	122.59
2	H	900	TPP	O2B-PB-O1B	2.57	118.84	110.58
2	A	900	TPP	CM2-C2'-N1'	2.65	120.21	117.03
2	E	900	TPP	C6'-N1'-C2'	2.67	120.43	115.77
2	C	900	TPP	C5-C4-N3	2.75	113.75	107.69
2	B	900	TPP	C5-C4-N3	2.79	113.84	107.69
2	F	900	TPP	C5-C4-N3	2.83	113.92	107.69
2	G	900	TPP	CM2-C2'-N1'	2.90	120.51	117.03
2	D	900	TPP	C5-C4-N3	2.91	114.09	107.69
2	B	900	TPP	O3B-PB-O3A	2.92	118.33	105.09
2	H	900	TPP	C6'-N1'-C2'	2.93	120.89	115.77
2	A	900	TPP	C6'-N1'-C2'	3.03	121.06	115.77
2	B	900	TPP	CM2-C2'-N3'	3.03	122.37	117.20
2	F	900	TPP	CM2-C2'-N3'	3.19	122.62	117.20
2	A	900	TPP	C5-C4-N3	3.19	114.71	107.69
2	D	900	TPP	CM2-C2'-N1'	3.19	120.86	117.03
2	D	900	TPP	C6'-N1'-C2'	3.20	121.36	115.77
2	B	900	TPP	N4'-C4'-N3'	3.27	121.69	116.95
2	G	900	TPP	O2A-PA-O3A	3.34	120.25	105.09
2	C	900	TPP	O3A-PA-O7	3.41	111.97	102.94
2	E	900	TPP	C5-C4-N3	3.56	115.53	107.69
2	F	900	TPP	C6'-N1'-C2'	4.10	122.94	115.77
2	D	900	TPP	C6'-C5'-C4'	4.15	121.68	115.72
2	G	900	TPP	C6'-N1'-C2'	4.27	123.24	115.77
2	C	900	TPP	C6'-N1'-C2'	4.63	123.86	115.77
2	B	900	TPP	C6'-N1'-C2'	5.24	124.92	115.77
2	B	900	TPP	C6-C5-C4	5.31	132.32	127.56
2	C	900	TPP	C6-C5-C4	5.38	132.39	127.56
2	F	900	TPP	C6-C5-C4	5.41	132.41	127.56
2	E	900	TPP	C6-C5-C4	6.41	133.31	127.56
2	D	900	TPP	C6-C5-C4	6.45	133.35	127.56
2	A	900	TPP	C6-C5-C4	7.48	134.27	127.56
2	G	900	TPP	C6-C5-C4	7.93	134.67	127.56
2	H	900	TPP	C6-C5-C4	9.27	135.88	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	TPP	4	0
2	B	900	TPP	3	0
2	C	900	TPP	2	0
2	D	900	TPP	2	0
2	E	900	TPP	3	0
2	F	900	TPP	3	0
2	G	900	TPP	1	0
2	H	900	TPP	5	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	813/831 (97%)	-0.36	19 (2%) 64 63	10, 18, 34, 88	0
1	B	813/831 (97%)	-0.32	19 (2%) 64 63	10, 19, 35, 91	0
1	C	813/831 (97%)	-0.16	29 (3%) 46 45	12, 21, 35, 94	0
1	D	813/831 (97%)	-0.28	16 (1%) 68 67	13, 22, 37, 84	0
1	E	813/831 (97%)	-0.15	33 (4%) 41 39	11, 22, 42, 93	0
1	F	813/831 (97%)	-0.12	34 (4%) 40 39	12, 23, 40, 85	0
1	G	813/831 (97%)	-0.33	18 (2%) 65 64	10, 21, 41, 97	0
1	H	813/831 (97%)	-0.21	17 (2%) 67 65	12, 24, 42, 85	0
All	All	6504/6648 (97%)	-0.24	185 (2%) 56 55	10, 21, 39, 97	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	814	VAL	8.1
1	C	812	GLY	7.3
1	G	811	LYS	7.2
1	C	813	ALA	7.0
1	F	814	VAL	6.9
1	G	812	GLY	6.8
1	G	814	VAL	6.7
1	B	814	VAL	6.5
1	F	809	ASP	6.4
1	A	814	VAL	6.2
1	E	814	VAL	6.1
1	B	812	GLY	6.1
1	D	814	VAL	6.1
1	C	814	VAL	6.1
1	G	809	ASP	6.0
1	C	809	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	811	LYS	5.7
1	F	813	ALA	5.6
1	G	813	ALA	5.6
1	F	812	GLY	5.4
1	B	811	LYS	5.1
1	B	813	ALA	5.1
1	H	809	ASP	4.9
1	E	811	LYS	4.7
1	E	812	GLY	4.7
1	E	808	THR	4.6
1	E	809	ASP	4.4
1	F	811	LYS	4.4
1	F	808	THR	4.2
1	F	157	LEU	4.1
1	D	811	LYS	4.1
1	A	808	THR	4.0
1	D	812	GLY	3.9
1	D	813	ALA	3.9
1	C	157	LEU	3.8
1	F	507	VAL	3.8
1	G	810	LYS	3.8
1	E	504	PHE	3.7
1	D	507	VAL	3.6
1	A	811	LYS	3.6
1	F	159	TYR	3.6
1	E	813	ALA	3.5
1	E	772	ASP	3.5
1	C	508	ILE	3.4
1	H	813	ALA	3.4
1	A	810	LYS	3.4
1	A	809	ASP	3.4
1	G	808	THR	3.4
1	D	809	ASP	3.4
1	C	507	VAL	3.3
1	H	507	VAL	3.3
1	B	808	THR	3.3
1	C	158	GLY	3.3
1	G	807	ASN	3.3
1	F	158	GLY	3.2
1	H	508	ILE	3.2
1	B	809	ASP	3.2
1	E	507	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	561	VAL	3.2
1	H	811	LYS	3.1
1	G	400	ALA	3.1
1	C	159	TYR	3.1
1	C	189	PRO	3.1
1	E	390	ASN	3.1
1	B	505	VAL	3.1
1	D	508	ILE	3.0
1	E	400	ALA	3.0
1	G	508	ILE	3.0
1	D	561	VAL	3.0
1	G	504	PHE	3.0
1	F	352	ALA	3.0
1	E	776	GLU	3.0
1	B	508	ILE	3.0
1	F	508	ILE	3.0
1	E	503	SER	3.0
1	H	808	THR	2.9
1	A	813	ALA	2.9
1	G	507	VAL	2.9
1	E	189	PRO	2.8
1	D	505	VAL	2.8
1	G	402	TYR	2.8
1	E	664	GLU	2.8
1	C	187	THR	2.8
1	C	772	ASP	2.8
1	A	812	GLY	2.7
1	E	508	ILE	2.7
1	H	157	LEU	2.7
1	A	772	ASP	2.7
1	F	477	LEU	2.7
1	F	810	LYS	2.7
1	C	190	LEU	2.6
1	A	507	VAL	2.6
1	F	511	MET	2.6
1	G	505	VAL	2.6
1	H	768	ASP	2.6
1	F	390	ASN	2.6
1	C	510	SER	2.6
1	A	775	ASP	2.6
1	F	154	GLY	2.6
1	B	507	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	808	THR	2.5
1	E	552	SER	2.5
1	B	504	PHE	2.5
1	C	768	ASP	2.5
1	E	506	HIS	2.5
1	C	561	VAL	2.5
1	A	329	ASP	2.4
1	F	187	THR	2.4
1	E	157	LEU	2.4
1	F	2	THR	2.4
1	B	159	TYR	2.4
1	E	810	LYS	2.4
1	C	767	ALA	2.4
1	F	189	PRO	2.4
1	E	775	ASP	2.4
1	C	512	LEU	2.3
1	E	665	LEU	2.3
1	F	512	LEU	2.3
1	C	180	VAL	2.3
1	F	504	PHE	2.3
1	A	157	LEU	2.3
1	A	512	LEU	2.3
1	C	390	ASN	2.3
1	D	389	PRO	2.3
1	B	561	VAL	2.3
1	H	696	ALA	2.3
1	B	512	LEU	2.3
1	F	50	GLU	2.3
1	B	187	THR	2.3
1	F	561	VAL	2.3
1	H	812	GLY	2.3
1	D	504	PHE	2.3
1	H	187	THR	2.2
1	G	561	VAL	2.2
1	E	551	PHE	2.2
1	B	157	LEU	2.2
1	C	155	GLY	2.2
1	D	808	THR	2.2
1	D	506	HIS	2.2
1	E	549	ASN	2.2
1	G	401	GLU	2.2
1	A	807	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	505	VAL	2.2
1	B	775	ASP	2.2
1	F	160	ALA	2.2
1	B	768	ASP	2.2
1	H	189	PRO	2.2
1	D	390	ASN	2.2
1	E	638	ASP	2.1
1	A	505	VAL	2.1
1	C	558	VAL	2.1
1	E	787	PHE	2.1
1	E	807	ASN	2.1
1	A	506	HIS	2.1
1	C	160	ALA	2.1
1	A	508	ILE	2.1
1	F	155	GLY	2.1
1	F	514	GLN	2.1
1	F	402	TYR	2.1
1	C	154	GLY	2.1
1	F	807	ASN	2.1
1	F	505	VAL	2.1
1	F	478	SER	2.1
1	C	401	GLU	2.1
1	G	551	PHE	2.1
1	A	557	GLY	2.1
1	E	767	ALA	2.1
1	E	635	LYS	2.1
1	D	392	GLU	2.1
1	B	480	HIS	2.1
1	E	758	THR	2.1
1	F	192	THR	2.1
1	H	511	MET	2.1
1	C	480	HIS	2.1
1	D	189	PRO	2.1
1	E	505	VAL	2.0
1	H	358	ASP	2.0
1	F	161	LEU	2.0
1	B	158	GLY	2.0
1	E	550	GLY	2.0
1	E	633	THR	2.0
1	F	156	GLU	2.0
1	G	157	LEU	2.0
1	H	512	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	510	SER	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	TPP	F	900	26/26	0.98	0.21	0.22	16,21,25,26	0
2	TPP	D	900	26/26	0.98	0.17	0.18	12,16,24,26	0
2	TPP	A	900	26/26	0.99	0.18	0.10	11,15,19,19	0
2	TPP	H	900	26/26	0.98	0.17	0.04	12,21,26,27	0
2	TPP	E	900	26/26	0.99	0.20	0.01	12,18,23,25	0
2	TPP	C	900	26/26	0.98	0.19	-0.01	14,19,24,25	0
2	TPP	G	900	26/26	0.99	0.16	-0.01	12,17,19,22	0
2	TPP	B	900	26/26	0.99	0.16	-0.12	11,16,19,19	0
3	CA	B	901	1/1	1.00	0.09	-1.16	13,13,13,13	0
3	CA	H	901	1/1	1.00	0.09	-1.28	14,14,14,14	0
3	CA	A	901	1/1	1.00	0.08	-1.50	10,10,10,10	0
3	CA	D	901	1/1	0.99	0.08	-1.53	12,12,12,12	0
3	CA	F	901	1/1	1.00	0.08	-1.77	13,13,13,13	0
3	CA	E	901	1/1	0.99	0.10	-1.84	12,12,12,12	0
3	CA	C	901	1/1	1.00	0.08	-2.13	12,12,12,12	0
3	CA	G	901	1/1	1.00	0.08	-2.16	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.