



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 06:16 PM EST

PDB ID : 2VBI  
Title : Holostructure of pyruvate decarboxylase from *Acetobacter pasteurianus*  
Authors : Gocke, D.; Berthold, C.L.; Schneider, G.; Pohl, M.  
Deposited on : 2007-09-14  
Resolution : 2.75 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

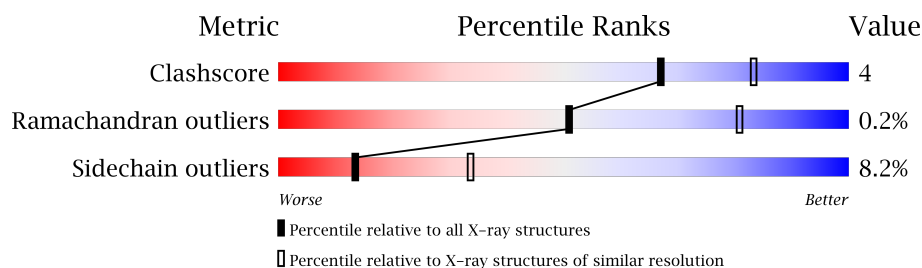
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	
1	B	566	
1	C	566	
1	D	566	
1	E	566	
1	F	566	
1	G	566	

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Mol	Chain	Length	Quality of chain
1	H	566	<div><div></div><div>83%</div><div>13%</div><div>..</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33860 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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	B	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	C	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	D	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	E	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	F	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	G	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			
1	H	554	Total	C	N	O	S	0	1	0
			4194	2637	731	801	25			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	GLY	conflict	UNP Q8L388
A	207	GLU	LYS	conflict	UNP Q8L388
A	208	LYS	ASN	conflict	UNP Q8L388
A	209	SER	ARG	conflict	UNP Q8L388
A	210	ALA	PRO	conflict	UNP Q8L388
A	211	SER	ALA	conflict	UNP Q8L388
A	297	ALA	GLY	conflict	UNP Q8L388
A	298	TRP	MET	conflict	UNP Q8L388
A	397	PRO	ALA	conflict	UNP Q8L388
B	25	ALA	GLY	conflict	UNP Q8L388
B	207	GLU	LYS	conflict	UNP Q8L388
B	208	LYS	ASN	conflict	UNP Q8L388
B	209	SER	ARG	conflict	UNP Q8L388

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Chain	Residue	Modelled	Actual	Comment	Reference
B	210	ALA	PRO	conflict	UNP Q8L388
B	211	SER	ALA	conflict	UNP Q8L388
B	297	ALA	GLY	conflict	UNP Q8L388
B	298	TRP	MET	conflict	UNP Q8L388
B	397	PRO	ALA	conflict	UNP Q8L388
C	25	ALA	GLY	conflict	UNP Q8L388
C	207	GLU	LYS	conflict	UNP Q8L388
C	208	LYS	ASN	conflict	UNP Q8L388
C	209	SER	ARG	conflict	UNP Q8L388
C	210	ALA	PRO	conflict	UNP Q8L388
C	211	SER	ALA	conflict	UNP Q8L388
C	297	ALA	GLY	conflict	UNP Q8L388
C	298	TRP	MET	conflict	UNP Q8L388
C	397	PRO	ALA	conflict	UNP Q8L388
D	25	ALA	GLY	conflict	UNP Q8L388
D	207	GLU	LYS	conflict	UNP Q8L388
D	208	LYS	ASN	conflict	UNP Q8L388
D	209	SER	ARG	conflict	UNP Q8L388
D	210	ALA	PRO	conflict	UNP Q8L388
D	211	SER	ALA	conflict	UNP Q8L388
D	297	ALA	GLY	conflict	UNP Q8L388
D	298	TRP	MET	conflict	UNP Q8L388
D	397	PRO	ALA	conflict	UNP Q8L388
E	25	ALA	GLY	conflict	UNP Q8L388
E	207	GLU	LYS	conflict	UNP Q8L388
E	208	LYS	ASN	conflict	UNP Q8L388
E	209	SER	ARG	conflict	UNP Q8L388
E	210	ALA	PRO	conflict	UNP Q8L388
E	211	SER	ALA	conflict	UNP Q8L388
E	297	ALA	GLY	conflict	UNP Q8L388
E	298	TRP	MET	conflict	UNP Q8L388
E	397	PRO	ALA	conflict	UNP Q8L388
F	25	ALA	GLY	conflict	UNP Q8L388
F	207	GLU	LYS	conflict	UNP Q8L388
F	208	LYS	ASN	conflict	UNP Q8L388
F	209	SER	ARG	conflict	UNP Q8L388
F	210	ALA	PRO	conflict	UNP Q8L388
F	211	SER	ALA	conflict	UNP Q8L388
F	297	ALA	GLY	conflict	UNP Q8L388
F	298	TRP	MET	conflict	UNP Q8L388
F	397	PRO	ALA	conflict	UNP Q8L388
G	25	ALA	GLY	conflict	UNP Q8L388

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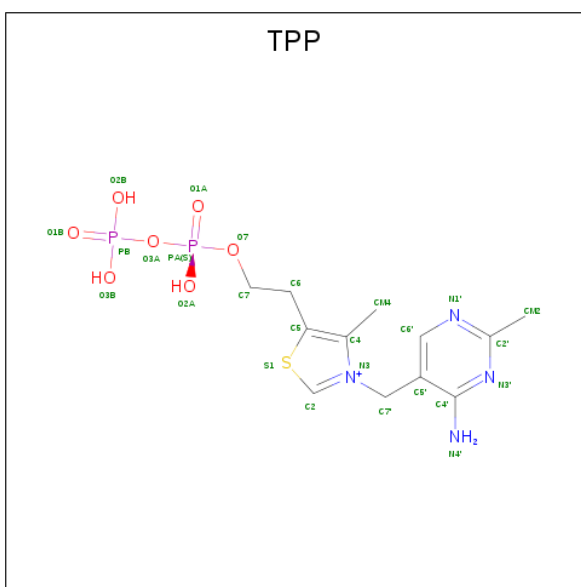
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Chain	Residue	Modelled	Actual	Comment	Reference
G	207	GLU	LYS	conflict	UNP Q8L388
G	208	LYS	ASN	conflict	UNP Q8L388
G	209	SER	ARG	conflict	UNP Q8L388
G	210	ALA	PRO	conflict	UNP Q8L388
G	211	SER	ALA	conflict	UNP Q8L388
G	297	ALA	GLY	conflict	UNP Q8L388
G	298	TRP	MET	conflict	UNP Q8L388
G	397	PRO	ALA	conflict	UNP Q8L388
H	25	ALA	GLY	conflict	UNP Q8L388
H	207	GLU	LYS	conflict	UNP Q8L388
H	208	LYS	ASN	conflict	UNP Q8L388
H	209	SER	ARG	conflict	UNP Q8L388
H	210	ALA	PRO	conflict	UNP Q8L388
H	211	SER	ALA	conflict	UNP Q8L388
H	297	ALA	GLY	conflict	UNP Q8L388
H	298	TRP	MET	conflict	UNP Q8L388
H	397	PRO	ALA	conflict	UNP Q8L388

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 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
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	E	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	F	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	G	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	H	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	5	Total O 5 5	0	0
4	C	14	Total O 14 14	0	0
4	D	15	Total O 15 15	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	20	Total 20	O 20	0	0
4	F	8	Total 8	O 8	0	0
4	G	11	Total 11	O 11	0	0
4	H	13	Total 13	O 13	0	0

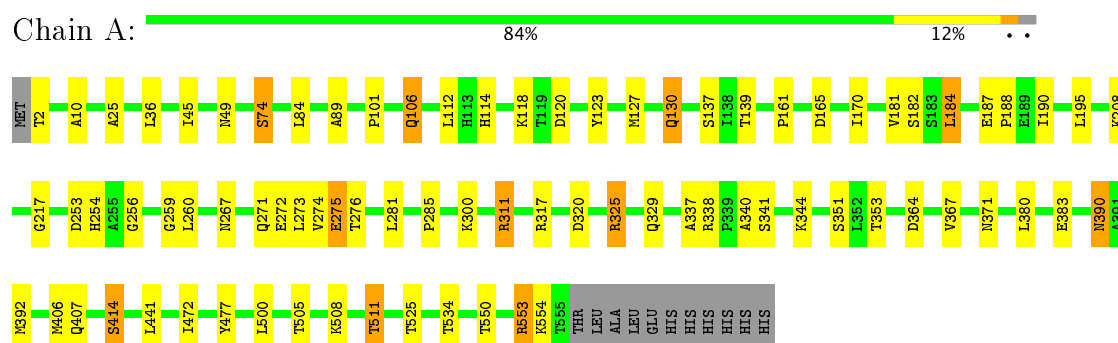


### 3 Residue-property plots

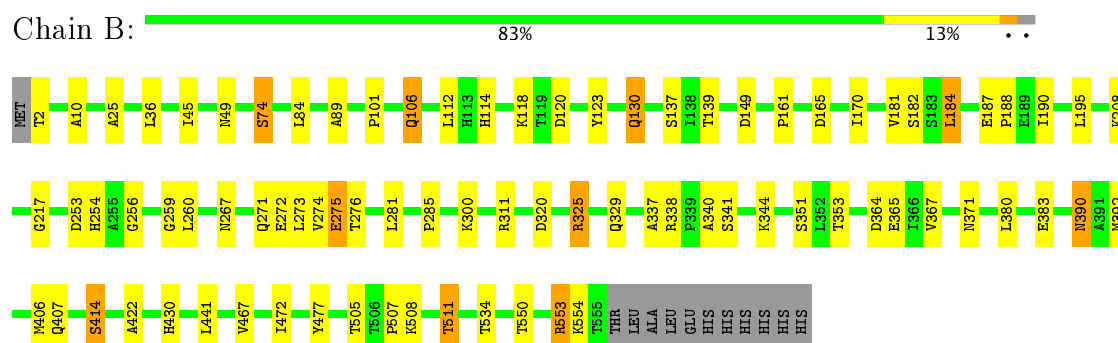
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

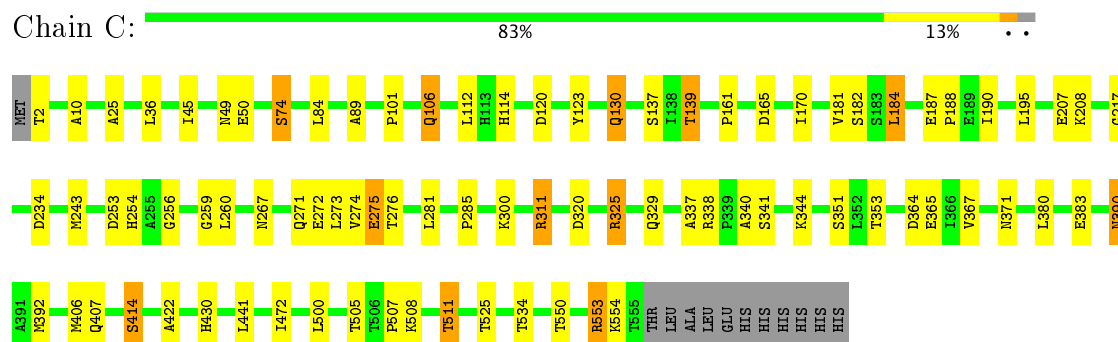
#### • Molecule 1: PYRUVATE DECARBOXYLASE

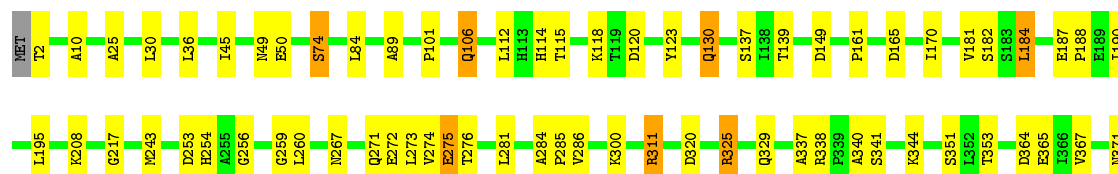


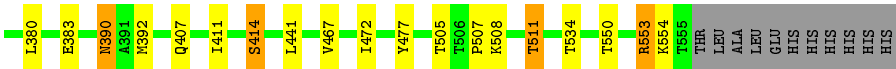
#### • Molecule 1: PYRUVATE DECARBOXYLASE



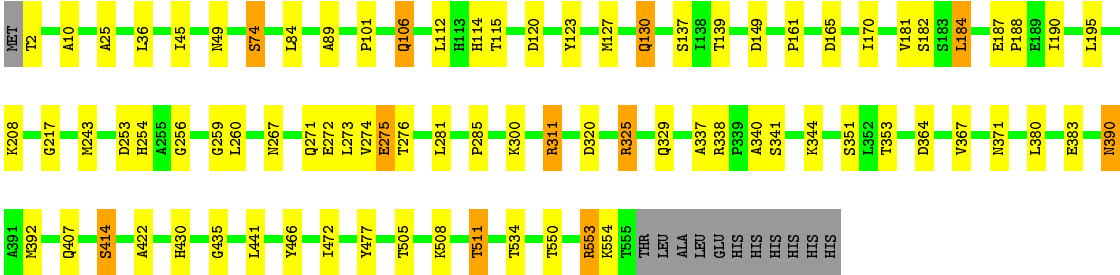
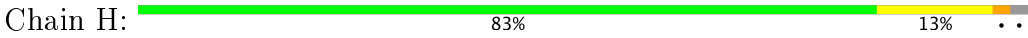
#### • Molecule 1: PYRUVATE DECARBOXYLASE







● Molecule 1: PYRUVATE DECARBOXYLASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.62Å 162.43Å 169.33Å 90.00° 102.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75	Depositor
% Data completeness (in resolution range)	97.1 (30.00-2.75)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	33860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.41	0/4282	0.55	0/5829
1	B	0.42	0/4282	0.55	0/5829
1	C	0.45	0/4282	0.56	0/5829
1	D	0.46	0/4282	0.57	0/5829
1	E	0.46	0/4282	0.58	0/5829
1	F	0.45	0/4282	0.57	0/5829
1	G	0.42	0/4282	0.56	0/5829
1	H	0.43	0/4282	0.55	0/5829
All	All	0.44	0/34256	0.56	0/46632

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4194	0	4148	39	0
1	B	4194	0	4148	38	0
1	C	4194	0	4148	42	0
1	D	4194	0	4148	44	2
1	E	4194	0	4148	46	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4194	0	4148	51	1
1	G	4194	0	4148	43	0
1	H	4194	0	4148	43	0
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
3	A	26	0	16	1	0
3	B	26	0	16	3	0
3	C	26	0	16	0	0
3	D	26	0	16	1	0
3	E	26	0	16	1	0
3	F	26	0	16	1	0
3	G	26	0	16	2	0
3	H	26	0	16	3	0
4	A	6	0	0	1	0
4	B	5	0	0	1	0
4	C	14	0	0	3	0
4	D	15	0	0	1	0
4	E	20	0	0	2	0
4	F	8	0	0	2	0
4	G	11	0	0	1	0
4	H	13	0	0	2	0
All	All	33860	0	33312	300	2

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 4.

All (300) 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:D:137:SER:HA	1:D:165:ASP:HB2	1.47	0.96
1:E:137:SER:HA	1:E:165:ASP:HB2	1.49	0.95
1:G:137:SER:HA	1:G:165:ASP:HB2	1.48	0.95
1:B:137:SER:HA	1:B:165:ASP:HB2	1.50	0.94
1:A:137:SER:HA	1:A:165:ASP:HB2	1.49	0.92
1:C:137:SER:HA	1:C:165:ASP:HB2	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:SER:HA	1:F:165:ASP:HB2	1.48	0.91
1:H:137:SER:HA	1:H:165:ASP:HB2	1.50	0.91
1:C:254:HIS:HD2	1:C:256:GLY:H	1.23	0.87
1:E:243:MET:CE	4:E:2007:HOH:O	2.24	0.85
1:G:254:HIS:HD2	1:G:256:GLY:H	1.24	0.84
1:E:254:HIS:HD2	1:E:256:GLY:H	1.26	0.83
1:H:243:MET:CE	4:H:2005:HOH:O	2.26	0.83
1:B:254:HIS:HD2	1:B:256:GLY:H	1.26	0.82
1:F:254:HIS:HD2	1:F:256:GLY:H	1.28	0.81
1:H:254:HIS:HD2	1:H:256:GLY:H	1.26	0.81
1:A:254:HIS:HD2	1:A:256:GLY:H	1.28	0.80
1:D:254:HIS:HD2	1:D:256:GLY:H	1.28	0.79
1:E:188:PRO:HA	1:H:188:PRO:HA	1.66	0.78
1:B:106:GLN:HG2	1:D:106:GLN:HG2	1.67	0.76
1:A:337:ALA:HB2	1:F:427:ASP:HB2	1.69	0.74
1:B:188:PRO:HA	1:C:188:PRO:HA	1.72	0.72
1:C:254:HIS:CD2	1:C:256:GLY:H	2.08	0.72
1:C:243:MET:CE	4:C:2006:HOH:O	2.38	0.71
1:C:260:LEU:HD13	1:C:392:MET:HE2	1.74	0.70
1:H:260:LEU:HD13	1:H:392:MET:HE2	1.72	0.70
1:G:254:HIS:CD2	1:G:256:GLY:H	2.09	0.70
1:D:192:HIS:CD2	1:F:192:HIS:CE1	2.80	0.69
1:H:243:MET:HE2	4:H:2005:HOH:O	1.92	0.69
1:F:106:GLN:HG2	1:H:106:GLN:HG2	1.73	0.68
1:F:243:MET:CE	4:F:2003:HOH:O	2.41	0.68
1:B:254:HIS:CD2	1:B:256:GLY:H	2.11	0.68
1:D:84:LEU:HD22	1:D:161:PRO:HB2	1.75	0.68
1:A:260:LEU:HD13	1:A:392:MET:HE2	1.76	0.68
1:H:254:HIS:CD2	1:H:256:GLY:H	2.10	0.67
1:A:254:HIS:CD2	1:A:256:GLY:H	2.12	0.67
1:F:254:HIS:CD2	1:F:256:GLY:H	2.12	0.67
1:E:260:LEU:HD13	1:E:392:MET:HE2	1.76	0.67
1:C:84:LEU:HD22	1:C:161:PRO:HB2	1.77	0.66
1:E:254:HIS:CD2	1:E:256:GLY:H	2.12	0.66
1:G:84:LEU:HD22	1:G:161:PRO:HB2	1.77	0.66
1:F:84:LEU:HD22	1:F:161:PRO:HB2	1.77	0.66
1:G:260:LEU:HD13	1:G:392:MET:HE2	1.78	0.65
1:A:84:LEU:HD22	1:A:161:PRO:HB2	1.78	0.65
1:B:84:LEU:HD22	1:B:161:PRO:HB2	1.78	0.65
1:E:207:GLU:O	1:E:338:ARG:NH2	2.29	0.65
1:E:84:LEU:HD22	1:E:161:PRO:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:LEU:HD22	1:H:161:PRO:HB2	1.78	0.65
1:D:254:HIS:CD2	1:D:256:GLY:H	2.13	0.64
1:F:188:PRO:HA	1:G:188:PRO:HA	1.80	0.64
1:D:260:LEU:HD13	1:D:392:MET:HE2	1.80	0.64
1:C:383:GLU:OE2	1:C:414:SER:HB2	1.97	0.64
1:E:106:GLN:HG2	1:G:106:GLN:HG2	1.80	0.64
1:F:260:LEU:HD13	1:F:392:MET:HE2	1.80	0.63
1:D:383:GLU:OE2	1:D:414:SER:HB2	1.99	0.63
1:A:383:GLU:OE2	1:A:414:SER:HB2	1.99	0.62
1:B:383:GLU:OE2	1:B:414:SER:HB2	1.99	0.62
1:G:353:THR:HG22	1:G:364:ASP:OD2	2.00	0.62
1:D:353:THR:HG22	1:D:364:ASP:OD2	1.99	0.61
1:E:383:GLU:OE2	1:E:414:SER:HB2	2.01	0.61
1:H:353:THR:HG22	1:H:364:ASP:OD2	2.01	0.61
1:B:353:THR:HG22	1:B:364:ASP:OD2	2.00	0.61
1:F:383:GLU:OE2	1:F:414:SER:HB2	2.00	0.61
1:A:353:THR:HG22	1:A:364:ASP:OD2	2.00	0.60
1:F:353:THR:HG22	1:F:364:ASP:OD2	2.00	0.60
1:B:101:PRO:HB3	1:B:112:LEU:HD13	1.82	0.60
1:B:260:LEU:HD13	1:B:392:MET:HE2	1.83	0.60
1:G:383:GLU:OE2	1:G:414:SER:HB2	2.02	0.60
1:H:383:GLU:OE2	1:H:414:SER:HB2	2.01	0.60
1:C:139:THR:HG22	4:C:2003:HOH:O	2.01	0.59
1:E:353:THR:HG22	1:E:364:ASP:OD2	2.03	0.59
1:C:353:THR:HG22	1:C:364:ASP:OD2	2.01	0.59
1:G:467:VAL:N	3:G:2000:TPP:O3B	2.36	0.58
1:A:101:PRO:HB3	1:A:112:LEU:HD13	1.85	0.58
1:C:101:PRO:HB3	1:C:112:LEU:HD13	1.86	0.58
1:H:101:PRO:HB3	1:H:112:LEU:HD13	1.85	0.58
3:B:2000:TPP:C2	3:B:2000:TPP:HN42	2.17	0.58
1:F:101:PRO:HB3	1:F:112:LEU:HD13	1.86	0.57
1:E:181:VAL:HG21	1:E:184:LEU:HD13	1.86	0.57
1:G:101:PRO:HB3	1:G:112:LEU:HD13	1.86	0.57
1:C:130:GLN:HG3	1:D:123:TYR:HB2	1.86	0.56
1:D:101:PRO:HB3	1:D:112:LEU:HD13	1.87	0.56
1:D:325:ARG:HH11	1:D:329:GLN:HE22	1.53	0.56
1:G:130:GLN:HG3	1:H:123:TYR:HB2	1.86	0.56
1:E:101:PRO:HB3	1:E:112:LEU:HD13	1.87	0.56
1:F:325:ARG:HH11	1:F:329:GLN:HE22	1.54	0.56
1:F:243:MET:HE2	4:F:2003:HOH:O	2.02	0.55
1:E:260:LEU:H	1:E:267:ASN:ND2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:TYR:HB2	1:D:130:GLN:HG3	1.88	0.55
1:E:243:MET:HE2	4:E:2007:HOH:O	2.01	0.55
1:E:325:ARG:HH11	1:E:329:GLN:HE22	1.53	0.54
1:A:106:GLN:HG2	1:C:106:GLN:HG2	1.90	0.54
1:E:123:TYR:HB2	1:F:130:GLN:HG3	1.90	0.54
1:H:325:ARG:HH11	1:H:329:GLN:HE22	1.54	0.54
1:C:49:ASN:HB3	1:D:441:LEU:HG	1.88	0.54
1:A:188:PRO:HA	1:D:188:PRO:HA	1.90	0.54
1:C:243:MET:HE2	4:C:2006:HOH:O	2.03	0.54
1:G:325:ARG:HH11	1:G:329:GLN:HE22	1.55	0.54
1:C:325:ARG:HH11	1:C:329:GLN:HE22	1.55	0.53
1:F:181:VAL:HG21	1:F:184:LEU:HD13	1.91	0.53
1:B:181:VAL:HG21	1:B:184:LEU:HD13	1.91	0.53
1:D:181:VAL:HG21	1:D:184:LEU:HD13	1.90	0.53
1:H:466:TYR:CD1	3:H:2000:TPP:H61	2.44	0.53
1:B:337:ALA:O	1:B:338:ARG:HD2	2.10	0.52
1:G:337:ALA:O	1:G:338:ARG:HD2	2.10	0.52
1:E:130:GLN:HG3	1:F:123:TYR:HB2	1.91	0.52
1:E:50:GLU:OE2	3:F:2000:TPP:N1'	2.42	0.52
1:A:89:ALA:HB1	1:A:407:GLN:HG3	1.92	0.52
1:A:181:VAL:HG21	1:A:184:LEU:HD13	1.91	0.52
1:A:337:ALA:O	1:A:338:ARG:HD2	2.10	0.52
1:G:118:LYS:NZ	4:G:2001:HOH:O	2.43	0.52
1:C:508:LYS:O	1:C:511:THR:HG22	2.10	0.51
1:A:508:LYS:O	1:A:511:THR:HG22	2.10	0.51
1:H:508:LYS:O	1:H:511:THR:HG22	2.10	0.51
1:H:337:ALA:O	1:H:338:ARG:HD2	2.10	0.51
1:G:508:LYS:O	1:G:511:THR:HG22	2.10	0.51
1:B:325:ARG:HH11	1:B:329:GLN:HE22	1.56	0.51
1:B:508:LYS:O	1:B:511:THR:HG22	2.10	0.51
1:E:508:LYS:O	1:E:511:THR:HG22	2.11	0.51
1:C:260:LEU:H	1:C:267:ASN:ND2	2.08	0.51
1:F:89:ALA:HB1	1:F:407:GLN:HG3	1.93	0.51
1:G:181:VAL:HG21	1:G:184:LEU:HD13	1.93	0.50
1:G:260:LEU:H	1:G:267:ASN:ND2	2.10	0.50
1:G:89:ALA:HB1	1:G:407:GLN:HG3	1.94	0.50
1:B:89:ALA:HB1	1:B:407:GLN:HG3	1.93	0.50
1:B:260:LEU:H	1:B:267:ASN:ND2	2.09	0.50
1:G:25:ALA:HB2	1:H:477:TYR:HB2	1.94	0.50
1:H:89:ALA:HB1	1:H:407:GLN:HG3	1.94	0.50
1:F:260:LEU:H	1:F:267:ASN:ND2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:441:LEU:HG	1:F:49:ASN:HB3	1.95	0.49
1:G:340:ALA:O	1:G:344:LYS:HD3	2.12	0.49
1:E:311:ARG:NH2	1:H:149:ASP:OD2	2.45	0.49
1:H:181:VAL:HG21	1:H:184:LEU:HD13	1.94	0.49
1:A:325:ARG:HH11	1:A:329:GLN:HE22	1.60	0.49
1:B:340:ALA:O	1:B:344:LYS:HD3	2.13	0.49
1:D:260:LEU:H	1:D:267:ASN:ND2	2.10	0.49
1:E:89:ALA:HB1	1:E:407:GLN:HG3	1.94	0.49
1:G:49:ASN:HB3	1:H:441:LEU:HG	1.94	0.49
1:D:337:ALA:O	1:D:338:ARG:HD2	2.11	0.49
1:A:260:LEU:H	1:A:267:ASN:ND2	2.09	0.49
1:A:311:ARG:NH2	1:D:149:ASP:OD2	2.46	0.49
1:A:25:ALA:HB2	1:B:477:TYR:HB2	1.95	0.49
1:A:340:ALA:O	1:A:344:LYS:HD3	2.13	0.48
1:C:337:ALA:O	1:C:338:ARG:HD2	2.13	0.48
1:F:508:LYS:O	1:F:511:THR:HG22	2.13	0.48
1:B:271:GLN:O	1:B:275:GLU:HB2	2.14	0.48
1:G:123:TYR:HB2	1:H:130:GLN:HG3	1.96	0.48
1:A:441:LEU:HG	1:B:49:ASN:HB3	1.96	0.48
1:B:467:VAL:N	3:B:2000:TPP:O3B	2.44	0.48
1:E:337:ALA:O	1:E:338:ARG:HD2	2.14	0.48
1:F:10:ALA:HB2	1:F:36:LEU:HD23	1.95	0.48
1:C:181:VAL:HG21	1:C:184:LEU:HD13	1.94	0.47
1:E:477:TYR:HB2	1:F:25:ALA:HB2	1.95	0.47
1:G:411:ILE:HD13	3:G:2000:TPP:HM42	1.97	0.47
1:C:367:VAL:HG22	1:C:390:ASN:HB2	1.96	0.47
1:H:260:LEU:H	1:H:267:ASN:ND2	2.12	0.47
1:H:340:ALA:O	1:H:344:LYS:HD3	2.14	0.47
1:H:217:GLY:HA3	1:H:285:PRO:HA	1.97	0.47
1:D:532:ASP:OD1	1:D:534:THR:HB	2.15	0.47
1:A:477:TYR:HB2	1:B:25:ALA:HB2	1.97	0.47
3:B:2000:TPP:HN42	3:B:2000:TPP:H2	1.77	0.47
1:F:337:ALA:O	1:F:338:ARG:HD2	2.14	0.47
1:B:367:VAL:HG22	1:B:390:ASN:HB2	1.96	0.47
1:E:367:VAL:HG22	1:E:390:ASN:HB2	1.97	0.47
1:C:130:GLN:HG2	1:D:127:MET:HG3	1.97	0.47
1:A:130:GLN:HG3	1:B:123:TYR:HB2	1.97	0.47
1:F:367:VAL:HG22	1:F:390:ASN:HB2	1.96	0.47
1:F:340:ALA:O	1:F:344:LYS:HD3	2.15	0.47
1:E:207:GLU:HA	1:E:336:PRO:HG3	1.96	0.46
1:E:49:ASN:HB3	1:F:441:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ALA:HB2	1:E:36:LEU:HD23	1.97	0.46
1:G:217:GLY:HA3	1:G:285:PRO:HA	1.97	0.46
1:A:367:VAL:HG22	1:A:390:ASN:HB2	1.97	0.46
1:A:49:ASN:HB3	1:B:441:LEU:HG	1.97	0.46
1:A:217:GLY:HA3	1:A:285:PRO:HA	1.97	0.46
1:B:118:LYS:NZ	4:B:2002:HOH:O	2.47	0.46
1:A:123:TYR:HB2	1:B:130:GLN:HG3	1.96	0.46
1:C:441:LEU:HG	1:D:49:ASN:HB3	1.98	0.46
1:C:10:ALA:HB2	1:C:36:LEU:HD23	1.97	0.46
1:D:340:ALA:O	1:D:344:LYS:HD3	2.16	0.46
1:D:89:ALA:HB1	1:D:407:GLN:HG3	1.97	0.46
1:H:367:VAL:HG22	1:H:390:ASN:HB2	1.97	0.46
1:C:89:ALA:HB1	1:C:407:GLN:HG3	1.97	0.46
1:F:311:ARG:NH2	1:G:149:ASP:OD2	2.49	0.46
1:H:550:THR:O	1:H:553:ARG:HB3	2.15	0.46
1:A:271:GLN:O	1:A:275:GLU:HB2	2.16	0.46
1:B:217:GLY:HA3	1:B:285:PRO:HA	1.97	0.46
1:E:340:ALA:O	1:E:344:LYS:HD3	2.15	0.46
1:G:10:ALA:HB2	1:G:36:LEU:HD23	1.97	0.46
1:D:10:ALA:HB2	1:D:36:LEU:HD23	1.98	0.45
1:D:74:SER:HB2	1:D:114:HIS:O	2.17	0.45
1:D:508:LYS:O	1:D:511:THR:HG22	2.15	0.45
3:A:2000:TPP:HN42	3:A:2000:TPP:C2	2.29	0.45
1:D:367:VAL:HG22	1:D:390:ASN:HB2	1.96	0.45
1:F:217:GLY:HA3	1:F:285:PRO:HA	1.97	0.45
1:E:308:GLU:HB3	1:E:309:PRO:CD	2.47	0.45
1:D:550:THR:O	1:D:553:ARG:HB3	2.16	0.45
1:F:532:ASP:OD1	1:F:534:THR:HB	2.17	0.45
1:D:192:HIS:HB3	1:F:192:HIS:CD2	2.52	0.45
1:A:118:LYS:NZ	4:A:2002:HOH:O	2.47	0.45
1:D:259:GLY:HA3	1:D:267:ASN:HD22	1.82	0.45
1:G:367:VAL:HG22	1:G:390:ASN:HB2	1.99	0.45
1:H:74:SER:HB2	1:H:114:HIS:O	2.16	0.45
1:A:550:THR:O	1:A:553:ARG:HB3	2.17	0.45
1:F:106:GLN:HG2	1:H:106:GLN:CG	2.44	0.45
1:F:365:GLU:HG2	1:F:507:PRO:HG3	1.99	0.45
1:E:500:LEU:HB3	1:E:525:THR:HG23	1.99	0.44
1:D:192:HIS:CG	1:F:192:HIS:NE2	2.86	0.44
1:E:217:GLY:HA3	1:E:285:PRO:HA	2.00	0.44
1:B:550:THR:O	1:B:553:ARG:HB3	2.16	0.44
1:C:340:ALA:O	1:C:344:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:GLN:O	1:H:275:GLU:HB2	2.17	0.44
1:G:50:GLU:OE2	3:H:2000:TPP:N1'	2.51	0.44
1:B:10:ALA:HB2	1:B:36:LEU:HD23	1.98	0.44
1:F:106:GLN:CG	1:H:106:GLN:HG2	2.45	0.44
1:G:74:SER:HB2	1:G:114:HIS:O	2.18	0.44
1:D:217:GLY:HA3	1:D:285:PRO:HA	2.00	0.43
1:E:550:THR:O	1:E:553:ARG:HB3	2.18	0.43
1:F:271:GLN:O	1:F:275:GLU:HB2	2.17	0.43
1:H:10:ALA:HB2	1:H:36:LEU:HD23	2.00	0.43
1:H:422:ALA:HA	1:H:430:HIS:CE1	2.53	0.43
1:A:406:MET:HE3	1:A:406:MET:HB3	1.90	0.43
1:C:271:GLN:O	1:C:275:GLU:HB2	2.17	0.43
1:G:271:GLN:O	1:G:275:GLU:HB2	2.19	0.43
1:B:406:MET:HB3	1:B:406:MET:HE3	1.95	0.43
1:C:217:GLY:HA3	1:C:285:PRO:HA	1.99	0.43
1:F:422:ALA:HA	1:F:430:HIS:CE1	2.53	0.43
1:H:259:GLY:HA3	1:H:267:ASN:HD22	1.83	0.43
1:A:74:SER:HB2	1:A:114:HIS:O	2.17	0.43
1:C:550:THR:O	1:C:553:ARG:HB3	2.19	0.43
1:A:317:ARG:HG2	1:D:177:ARG:HB2	1.99	0.43
1:B:74:SER:HB2	1:B:114:HIS:O	2.19	0.43
1:B:149:ASP:OD2	1:C:311:ARG:NH2	2.52	0.43
1:C:259:GLY:HA3	1:C:267:ASN:HD22	1.84	0.43
1:E:25:ALA:HB2	1:F:477:TYR:HB2	2.01	0.43
1:G:30:LEU:HD22	1:H:477:TYR:CE1	2.54	0.43
1:F:259:GLY:HA3	1:F:267:ASN:HD22	1.83	0.43
1:A:10:ALA:HB2	1:A:36:LEU:HD23	2.00	0.42
1:D:184:LEU:HA	1:D:184:LEU:HD12	1.92	0.42
1:G:441:LEU:HG	1:H:49:ASN:HB3	2.01	0.42
1:G:550:THR:O	1:G:553:ARG:HB3	2.19	0.42
1:F:74:SER:HB2	1:F:114:HIS:O	2.19	0.42
1:A:337:ALA:CB	1:F:427:ASP:HB2	2.44	0.42
1:F:367:VAL:CG2	1:F:390:ASN:HB2	2.49	0.42
1:H:435:GLY:HA3	3:H:2000:TPP:O2A	2.19	0.42
1:D:190:ILE:C	1:D:190:ILE:HD13	2.40	0.42
1:C:25:ALA:HB2	1:D:477:TYR:HB2	2.00	0.42
1:F:550:THR:O	1:F:553:ARG:HB3	2.18	0.42
1:D:365:GLU:HG2	1:D:507:PRO:HG3	2.01	0.42
1:F:184:LEU:HA	1:F:184:LEU:HD12	1.92	0.42
1:A:259:GLY:HA3	1:A:267:ASN:HD22	1.84	0.42
1:D:367:VAL:CG2	1:D:390:ASN:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:ILE:O	1:F:81:MET:HB2	2.19	0.42
1:G:259:GLY:HA3	1:G:267:ASN:HD22	1.84	0.42
1:C:74:SER:HB2	1:C:114:HIS:O	2.19	0.42
1:D:422:ALA:HA	1:D:430:HIS:CE1	2.55	0.42
1:F:423:MET:HE2	1:F:454:LEU:HD21	2.02	0.42
1:C:207:GLU:O	1:C:338:ARG:NH2	2.52	0.42
1:E:184:LEU:HA	1:E:184:LEU:HD12	1.88	0.42
1:E:477:TYR:CE1	1:F:30:LEU:HD22	2.55	0.42
1:D:271:GLN:O	1:D:275:GLU:HB2	2.20	0.42
1:E:234:ASP:OD1	1:E:254:HIS:HE1	2.03	0.42
1:G:115:THR:HA	1:G:123:TYR:OH	2.20	0.42
1:B:367:VAL:CG2	1:B:390:ASN:HB2	2.50	0.41
1:E:423:MET:HE2	1:E:454:LEU:HD21	2.01	0.41
1:D:118:LYS:NZ	4:D:2004:HOH:O	2.47	0.41
1:G:284:ALA:N	1:G:285:PRO:CD	2.84	0.41
1:C:50:GLU:OE2	3:D:2000:TPP:N1'	2.53	0.41
1:G:477:TYR:HB2	1:H:25:ALA:HB2	2.03	0.41
3:E:2000:TPP:C2	3:E:2000:TPP:HN42	2.34	0.41
1:F:149:ASP:OD2	1:G:311:ARG:NH2	2.53	0.41
1:A:500:LEU:HB3	1:A:525:THR:HG23	2.03	0.41
1:C:500:LEU:HB3	1:C:525:THR:HG23	2.03	0.41
1:A:367:VAL:CG2	1:A:390:ASN:HB2	2.51	0.41
1:H:367:VAL:CG2	1:H:390:ASN:HB2	2.50	0.41
1:C:234:ASP:OD1	1:C:254:HIS:HE1	2.04	0.41
1:C:367:VAL:CG2	1:C:390:ASN:HB2	2.51	0.41
1:D:78:ILE:O	1:D:81:MET:HB2	2.21	0.41
1:E:203:VAL:HG21	1:E:334:LYS:HB2	2.02	0.41
1:A:127:MET:HG3	1:B:130:GLN:HG2	2.03	0.41
1:C:406:MET:HB3	1:C:406:MET:HE3	1.96	0.41
1:E:271:GLN:O	1:E:275:GLU:HB2	2.21	0.41
1:B:422:ALA:HA	1:B:430:HIS:CE1	2.56	0.41
1:C:365:GLU:HG2	1:C:507:PRO:HG3	2.03	0.41
1:F:500:LEU:HB3	1:F:525:THR:HG23	2.02	0.41
1:D:144:ALA:HB3	1:D:145:PRO:HD3	2.03	0.40
1:E:284:ALA:N	1:E:285:PRO:CD	2.85	0.40
1:E:149:ASP:OD2	1:H:311:ARG:NH2	2.55	0.40
1:E:365:GLU:HG2	1:E:507:PRO:HG3	2.03	0.40
1:E:532:ASP:OD1	1:E:534:THR:HB	2.21	0.40
1:E:74:SER:HB2	1:E:114:HIS:O	2.21	0.40
1:G:184:LEU:HD12	1:G:184:LEU:HA	1.94	0.40
1:H:115:THR:HA	1:H:123:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:GLN:HG2	1:H:127:MET:HG3	2.04	0.40
1:B:259:GLY:HA3	1:B:267:ASN:HD22	1.84	0.40
1:B:365:GLU:HG2	1:B:507:PRO:HG3	2.03	0.40
1:F:506:THR:OG1	1:F:509:GLU:HB2	2.22	0.40
1:G:365:GLU:HG2	1:G:507:PRO:HG3	2.03	0.40
1:C:422:ALA:HA	1:C:430:HIS:CE1	2.56	0.40
1:G:243:MET:HE1	1:G:286:VAL:H	1.86	0.40

All (2) 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:D:360:GLY:N	1:F:533:ARG:NH1[3_555]	1.95	0.25
1:D:509:GLU:OE2	1:E:496:GLU:CG[3_555]	2.09	0.11

## 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	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
1	B	553/566 (98%)	539 (98%)	13 (2%)	1 (0%)	51	81
1	C	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
1	D	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
1	E	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
1	F	553/566 (98%)	539 (98%)	13 (2%)	1 (0%)	51	81
1	G	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
1	H	553/566 (98%)	538 (97%)	14 (2%)	1 (0%)	51	81
All	All	4424/4528 (98%)	4306 (97%)	110 (2%)	8 (0%)	51	81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	SER
1	B	74	SER
1	C	74	SER
1	D	74	SER
1	E	74	SER
1	F	74	SER
1	G	74	SER
1	H	74	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	440/450 (98%)	404 (92%)	36 (8%)	13	34
1	B	440/450 (98%)	404 (92%)	36 (8%)	13	34
1	C	440/450 (98%)	404 (92%)	36 (8%)	13	34
1	D	440/450 (98%)	404 (92%)	36 (8%)	13	34
1	E	440/450 (98%)	405 (92%)	35 (8%)	14	35
1	F	440/450 (98%)	403 (92%)	37 (8%)	13	32
1	G	440/450 (98%)	404 (92%)	36 (8%)	13	34
1	H	440/450 (98%)	404 (92%)	36 (8%)	13	34
All	All	3520/3600 (98%)	3232 (92%)	288 (8%)	13	34

All (288) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	45	ILE
1	A	106	GLN
1	A	120	ASP
1	A	130	GLN
1	A	139	THR

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Mol	Chain	Res	Type
1	A	170	ILE
1	A	182	SER
1	A	184	LEU
1	A	187	GLU
1	A	190	ILE
1	A	195	LEU
1	A	208	LYS
1	A	253	ASP
1	A	272	GLU
1	A	273	LEU
1	A	274	VAL
1	A	275	GLU
1	A	276	THR
1	A	281	LEU
1	A	300	LYS
1	A	311	ARG
1	A	320	ASP
1	A	325	ARG
1	A	341	SER
1	A	351	SER
1	A	371	ASN
1	A	380	LEU
1	A	390	ASN
1	A	414	SER
1	A	472	ILE
1	A	505	THR
1	A	511	THR
1	A	534	THR
1	A	553	ARG
1	A	554	LYS
1	B	2	THR
1	B	45	ILE
1	B	106	GLN
1	B	120	ASP
1	B	130	GLN
1	B	139	THR
1	B	170	ILE
1	B	182	SER
1	B	184	LEU
1	B	187	GLU
1	B	190	ILE
1	B	195	LEU

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Mol	Chain	Res	Type
1	B	208	LYS
1	B	253	ASP
1	B	272	GLU
1	B	273	LEU
1	B	274	VAL
1	B	275	GLU
1	B	276	THR
1	B	281	LEU
1	B	300	LYS
1	B	311	ARG
1	B	320	ASP
1	B	325	ARG
1	B	341	SER
1	B	351	SER
1	B	371	ASN
1	B	380	LEU
1	B	390	ASN
1	B	414	SER
1	B	472	ILE
1	B	505	THR
1	B	511	THR
1	B	534	THR
1	B	553	ARG
1	B	554	LYS
1	C	2	THR
1	C	45	ILE
1	C	106	GLN
1	C	120	ASP
1	C	130	GLN
1	C	139	THR
1	C	170	ILE
1	C	182	SER
1	C	184	LEU
1	C	187	GLU
1	C	190	ILE
1	C	195	LEU
1	C	208	LYS
1	C	253	ASP
1	C	272	GLU
1	C	273	LEU
1	C	274	VAL
1	C	275	GLU

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Mol	Chain	Res	Type
1	C	276	THR
1	C	281	LEU
1	C	300	LYS
1	C	311	ARG
1	C	320	ASP
1	C	325	ARG
1	C	341	SER
1	C	351	SER
1	C	371	ASN
1	C	380	LEU
1	C	390	ASN
1	C	414	SER
1	C	472	ILE
1	C	505	THR
1	C	511	THR
1	C	534	THR
1	C	553	ARG
1	C	554	LYS
1	D	2	THR
1	D	45	ILE
1	D	106	GLN
1	D	120	ASP
1	D	130	GLN
1	D	139	THR
1	D	170	ILE
1	D	182	SER
1	D	184	LEU
1	D	187	GLU
1	D	190	ILE
1	D	195	LEU
1	D	208	LYS
1	D	253	ASP
1	D	272	GLU
1	D	273	LEU
1	D	274	VAL
1	D	275	GLU
1	D	276	THR
1	D	281	LEU
1	D	300	LYS
1	D	311	ARG
1	D	320	ASP
1	D	325	ARG

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Mol	Chain	Res	Type
1	D	341	SER
1	D	351	SER
1	D	371	ASN
1	D	380	LEU
1	D	390	ASN
1	D	414	SER
1	D	472	ILE
1	D	505	THR
1	D	511	THR
1	D	534	THR
1	D	553	ARG
1	D	554	LYS
1	E	2	THR
1	E	45	ILE
1	E	106	GLN
1	E	120	ASP
1	E	130	GLN
1	E	139	THR
1	E	170	ILE
1	E	182	SER
1	E	184	LEU
1	E	187	GLU
1	E	190	ILE
1	E	195	LEU
1	E	253	ASP
1	E	272	GLU
1	E	273	LEU
1	E	274	VAL
1	E	275	GLU
1	E	276	THR
1	E	281	LEU
1	E	300	LYS
1	E	311	ARG
1	E	320	ASP
1	E	325	ARG
1	E	341	SER
1	E	351	SER
1	E	371	ASN
1	E	380	LEU
1	E	390	ASN
1	E	414	SER
1	E	472	ILE

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Mol	Chain	Res	Type
1	E	505	THR
1	E	511	THR
1	E	534	THR
1	E	553	ARG
1	E	554	LYS
1	F	2	THR
1	F	45	ILE
1	F	106	GLN
1	F	120	ASP
1	F	130	GLN
1	F	139	THR
1	F	170	ILE
1	F	182	SER
1	F	184	LEU
1	F	187	GLU
1	F	190	ILE
1	F	195	LEU
1	F	208	LYS
1	F	253	ASP
1	F	268	PRO
1	F	272	GLU
1	F	273	LEU
1	F	274	VAL
1	F	275	GLU
1	F	276	THR
1	F	281	LEU
1	F	300	LYS
1	F	311	ARG
1	F	320	ASP
1	F	325	ARG
1	F	341	SER
1	F	351	SER
1	F	371	ASN
1	F	380	LEU
1	F	390	ASN
1	F	414	SER
1	F	472	ILE
1	F	505	THR
1	F	511	THR
1	F	534	THR
1	F	553	ARG
1	F	554	LYS

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Mol	Chain	Res	Type
1	G	2	THR
1	G	45	ILE
1	G	106	GLN
1	G	120	ASP
1	G	130	GLN
1	G	139	THR
1	G	170	ILE
1	G	182	SER
1	G	184	LEU
1	G	187	GLU
1	G	190	ILE
1	G	195	LEU
1	G	208	LYS
1	G	253	ASP
1	G	272	GLU
1	G	273	LEU
1	G	274	VAL
1	G	275	GLU
1	G	276	THR
1	G	281	LEU
1	G	300	LYS
1	G	311	ARG
1	G	320	ASP
1	G	325	ARG
1	G	341	SER
1	G	351	SER
1	G	371	ASN
1	G	380	LEU
1	G	390	ASN
1	G	414	SER
1	G	472	ILE
1	G	505	THR
1	G	511	THR
1	G	534	THR
1	G	553	ARG
1	G	554	LYS
1	H	2	THR
1	H	45	ILE
1	H	106	GLN
1	H	120	ASP
1	H	130	GLN
1	H	139	THR

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Mol	Chain	Res	Type
1	H	170	ILE
1	H	182	SER
1	H	184	LEU
1	H	187	GLU
1	H	190	ILE
1	H	195	LEU
1	H	208	LYS
1	H	253	ASP
1	H	272	GLU
1	H	273	LEU
1	H	274	VAL
1	H	275	GLU
1	H	276	THR
1	H	281	LEU
1	H	300	LYS
1	H	311	ARG
1	H	320	ASP
1	H	325	ARG
1	H	341	SER
1	H	351	SER
1	H	371	ASN
1	H	380	LEU
1	H	390	ASN
1	H	414	SER
1	H	472	ILE
1	H	505	THR
1	H	511	THR
1	H	534	THR
1	H	553	ARG
1	H	554	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	44	GLN
1	A	64	ASN
1	A	254	HIS
1	A	267	ASN
1	A	329	GLN
1	A	430	HIS
1	B	35	GLN

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Mol	Chain	Res	Type
1	B	44	GLN
1	B	64	ASN
1	B	254	HIS
1	B	267	ASN
1	B	329	GLN
1	C	35	GLN
1	C	44	GLN
1	C	64	ASN
1	C	254	HIS
1	C	267	ASN
1	C	329	GLN
1	C	430	HIS
1	D	35	GLN
1	D	44	GLN
1	D	64	ASN
1	D	192	HIS
1	D	254	HIS
1	D	267	ASN
1	D	329	GLN
1	D	430	HIS
1	E	35	GLN
1	E	44	GLN
1	E	64	ASN
1	E	254	HIS
1	E	267	ASN
1	E	329	GLN
1	E	430	HIS
1	F	35	GLN
1	F	44	GLN
1	F	64	ASN
1	F	192	HIS
1	F	254	HIS
1	F	267	ASN
1	F	329	GLN
1	F	363	ASN
1	F	430	HIS
1	G	35	GLN
1	G	44	GLN
1	G	64	ASN
1	G	237	GLN
1	G	254	HIS
1	G	267	ASN

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Mol	Chain	Res	Type
1	G	329	GLN
1	G	430	HIS
1	H	35	GLN
1	H	44	GLN
1	H	64	ASN
1	H	254	HIS
1	H	267	ASN
1	H	329	GLN
1	H	430	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	$\# Z  > 2$
3	TPP	A	2000	2	21,27,27	1.43	5 (23%)	25,40,40	1.83	7 (28%)
3	TPP	B	2000	2	21,27,27	1.42	4 (19%)	25,40,40	1.74	6 (24%)
3	TPP	C	2000	2	21,27,27	1.62	4 (19%)	25,40,40	1.72	7 (28%)
3	TPP	D	2000	2	21,27,27	1.32	4 (19%)	25,40,40	1.68	7 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TPP	E	2000	2	21,27,27	1.41	5 (23%)	25,40,40	1.63	8 (32%)
3	TPP	F	2000	2	21,27,27	1.47	4 (19%)	25,40,40	1.88	5 (20%)
3	TPP	G	2000	2	21,27,27	1.29	4 (19%)	25,40,40	1.79	7 (28%)
3	TPP	H	2000	2	21,27,27	1.36	5 (23%)	25,40,40	1.79	7 (28%)

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	TPP	A	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	B	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	C	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	D	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	E	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	F	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	G	2000	2	-	0/16/17/17	0/2/2/2
3	TPP	H	2000	2	-	0/16/17/17	0/2/2/2

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2000	TPP	C4-N3	-4.33	1.35	1.39
3	C	2000	TPP	C4-N3	-4.05	1.36	1.39
3	E	2000	TPP	C4-N3	-3.15	1.37	1.39
3	D	2000	TPP	C4-N3	-3.14	1.37	1.39
3	B	2000	TPP	C4-N3	-3.00	1.37	1.39
3	A	2000	TPP	C4-N3	-2.92	1.37	1.39
3	G	2000	TPP	C4-N3	-2.80	1.37	1.39
3	H	2000	TPP	C7'-N3	-2.36	1.44	1.48
3	H	2000	TPP	C4-N3	-2.31	1.37	1.39
3	A	2000	TPP	C7'-N3	-2.08	1.45	1.48
3	E	2000	TPP	C4'-N3'	2.05	1.38	1.35
3	E	2000	TPP	C2'-N1'	2.11	1.37	1.34
3	D	2000	TPP	C4'-N3'	2.11	1.38	1.35
3	F	2000	TPP	C2'-N1'	2.11	1.37	1.34
3	E	2000	TPP	C6'-N1'	2.12	1.39	1.34
3	G	2000	TPP	C2'-N3'	2.17	1.38	1.34
3	C	2000	TPP	C2'-N1'	2.19	1.38	1.34
3	H	2000	TPP	C2'-N1'	2.24	1.38	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2000	TPP	C4'-N3'	2.28	1.38	1.35
3	A	2000	TPP	C4'-N3'	2.30	1.38	1.35
3	F	2000	TPP	C2'-N3'	2.30	1.38	1.34
3	F	2000	TPP	C4'-N3'	2.32	1.38	1.35
3	B	2000	TPP	C4'-N3'	2.32	1.38	1.35
3	G	2000	TPP	C2'-N1'	2.39	1.38	1.34
3	B	2000	TPP	C2'-N1'	2.49	1.38	1.34
3	H	2000	TPP	C4'-N3'	2.52	1.38	1.35
3	E	2000	TPP	C2'-N3'	2.59	1.38	1.34
3	D	2000	TPP	C2'-N3'	2.60	1.38	1.34
3	H	2000	TPP	C2'-N3'	2.60	1.38	1.34
3	A	2000	TPP	C2'-N1'	2.62	1.38	1.34
3	B	2000	TPP	C2'-N3'	2.65	1.38	1.34
3	D	2000	TPP	C2'-N1'	2.67	1.38	1.34
3	A	2000	TPP	C2'-N3'	2.79	1.39	1.34
3	C	2000	TPP	C4'-N3'	2.98	1.39	1.35
3	C	2000	TPP	C2'-N3'	3.43	1.40	1.34

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2000	TPP	N1'-C2'-N3'	-3.42	119.67	125.59
3	E	2000	TPP	N1'-C2'-N3'	-3.25	119.97	125.59
3	D	2000	TPP	N1'-C2'-N3'	-3.21	120.03	125.59
3	B	2000	TPP	N1'-C2'-N3'	-3.19	120.06	125.59
3	G	2000	TPP	N1'-C2'-N3'	-2.93	120.52	125.59
3	F	2000	TPP	N1'-C2'-N3'	-2.91	120.55	125.59
3	A	2000	TPP	N1'-C2'-N3'	-2.86	120.63	125.59
3	C	2000	TPP	N1'-C2'-N3'	-2.86	120.64	125.59
3	D	2000	TPP	C5'-C6'-N1'	-2.55	119.56	123.87
3	G	2000	TPP	C5'-C6'-N1'	-2.30	119.97	123.87
3	A	2000	TPP	C5'-C6'-N1'	-2.30	119.98	123.87
3	C	2000	TPP	C5'-C4'-N4'	-2.14	119.11	122.22
3	E	2000	TPP	C5'-C6'-N1'	-2.11	120.30	123.87
3	H	2000	TPP	C5'-C6'-N1'	-2.08	120.35	123.87
3	D	2000	TPP	CM4-C4-C5	-2.02	123.39	127.29
3	E	2000	TPP	CM4-C4-C5	-2.01	123.39	127.29
3	C	2000	TPP	CM4-C4-N3	2.04	125.14	122.53
3	A	2000	TPP	CM2-C2'-N1'	2.10	119.43	117.06
3	E	2000	TPP	C6'-C5'-C4'	2.13	118.51	115.68
3	F	2000	TPP	CM2-C2'-N1'	2.18	119.52	117.06
3	H	2000	TPP	C6'-C5'-C4'	2.23	118.65	115.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2000	TPP	C6'-C5'-C4'	2.28	118.72	115.68
3	B	2000	TPP	C6'-N1'-C2'	2.29	119.84	115.88
3	D	2000	TPP	C6'-C5'-C4'	2.32	118.76	115.68
3	F	2000	TPP	C6'-N1'-C2'	2.32	119.89	115.88
3	C	2000	TPP	CM2-C2'-N3'	2.39	121.11	117.20
3	D	2000	TPP	CM2-C2'-N1'	2.44	119.81	117.06
3	B	2000	TPP	C6'-C5'-C4'	2.44	118.92	115.68
3	E	2000	TPP	CM2-C2'-N1'	2.46	119.83	117.06
3	A	2000	TPP	C6'-N1'-C2'	2.46	120.13	115.88
3	B	2000	TPP	CM2-C2'-N1'	2.54	119.93	117.06
3	G	2000	TPP	C6'-N1'-C2'	2.55	120.28	115.88
3	E	2000	TPP	C6'-N1'-C2'	2.58	120.34	115.88
3	E	2000	TPP	C6-C5-C4	2.60	129.52	127.43
3	B	2000	TPP	CM4-C4-N3	2.60	125.85	122.53
3	G	2000	TPP	C6'-C5'-C4'	2.63	119.17	115.68
3	C	2000	TPP	C6'-C5'-C4'	2.73	119.30	115.68
3	H	2000	TPP	C6'-N1'-C2'	2.86	120.82	115.88
3	A	2000	TPP	C6'-C5'-C4'	2.87	119.50	115.68
3	C	2000	TPP	N4'-C4'-N3'	3.01	121.44	117.00
3	H	2000	TPP	CM2-C2'-N1'	3.13	120.59	117.06
3	D	2000	TPP	C6'-N1'-C2'	3.18	121.38	115.88
3	H	2000	TPP	CM4-C4-N3	3.19	126.60	122.53
3	A	2000	TPP	CM4-C4-N3	3.47	126.95	122.53
3	E	2000	TPP	CM4-C4-N3	3.51	127.01	122.53
3	G	2000	TPP	CM2-C2'-N1'	3.51	121.03	117.06
3	G	2000	TPP	CM4-C4-N3	3.54	127.05	122.53
3	D	2000	TPP	CM4-C4-N3	3.82	127.40	122.53
3	G	2000	TPP	C6-C5-C4	4.00	130.64	127.43
3	C	2000	TPP	C6-C5-C4	4.49	131.04	127.43
3	H	2000	TPP	C6-C5-C4	4.50	131.04	127.43
3	B	2000	TPP	C6-C5-C4	4.81	131.29	127.43
3	A	2000	TPP	C6-C5-C4	5.07	131.50	127.43
3	F	2000	TPP	C6-C5-C4	6.57	132.71	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2000	TPP	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2000	TPP	3	0
3	D	2000	TPP	1	0
3	E	2000	TPP	1	0
3	F	2000	TPP	1	0
3	G	2000	TPP	2	0
3	H	2000	TPP	3	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.