



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1VPX  
Title : Crystal structure of Transaldolase (EC 2.2.1.2) (TM0295) from *Thermotoga maritima* at 2.40 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2004-11-23  
Resolution : 2.40 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

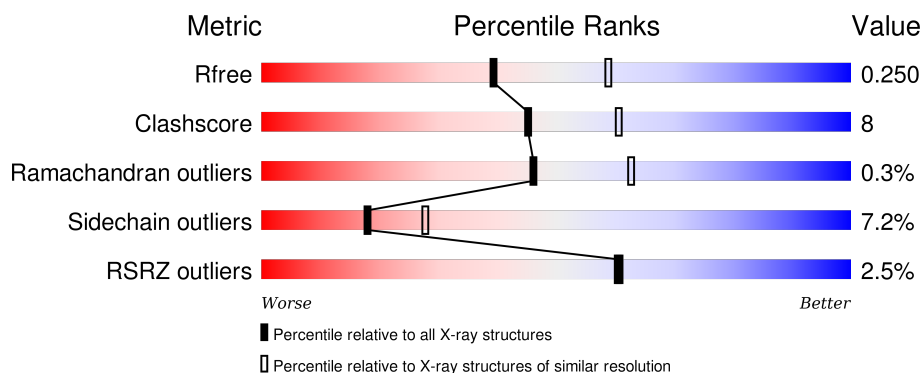
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	230	<div> <div>71%</div> <div>16%</div> <div>•</div> <div>10%</div> </div>
1	B	230	<div> <div>71%</div> <div>17%</div> <div>•</div> <div>9%</div> </div>
1	C	230	<div> <div>67%</div> <div>20%</div> <div>•</div> <div>10%</div> </div>
1	D	230	<div> <div>73%</div> <div>17%</div> <div>•</div> <div>9%</div> </div>
1	E	230	<div> <div>72%</div> <div>20%</div> <div>•</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
1	K	230	
1	L	230	
1	M	230	
1	N	230	
1	O	230	
1	P	230	
1	Q	230	
1	R	230	
1	S	230	
1	T	230	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	O	219	-	-	-	X
3	GOL	H	219	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31916 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 PROTEIN (Transaldolase (EC 2.2.1.2)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1591	1022	258	299	12			
1	B	209	Total	C	N	O	S	0	0	0
			1584	1016	260	296	12			
1	C	208	Total	C	N	O	S	0	0	0
			1560	997	252	299	12			
1	D	210	Total	C	N	O	S	0	0	0
			1615	1034	264	305	12			
1	E	216	Total	C	N	O	S	0	0	0
			1674	1075	272	315	12			
1	F	213	Total	C	N	O	S	0	0	0
			1655	1064	270	309	12			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1070	271	314	12			
1	H	205	Total	C	N	O	S	0	0	0
			1550	996	248	294	12			
1	I	211	Total	C	N	O	S	0	0	0
			1615	1034	264	305	12			
1	J	213	Total	C	N	O	S	0	0	0
			1619	1038	263	306	12			
1	K	216	Total	C	N	O	S	0	0	0
			1651	1059	265	315	12			
1	L	204	Total	C	N	O	S	0	0	0
			1530	980	249	289	12			
1	M	198	Total	C	N	O	S	0	0	0
			1457	928	240	278	11			
1	N	204	Total	C	N	O	S	0	0	0
			1475	939	243	281	12			
1	O	210	Total	C	N	O	S	0	0	0
			1604	1025	260	307	12			
1	P	209	Total	C	N	O	S	0	0	0
			1576	1010	258	296	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	208	Total	C	N	O	S	0	1	0
			1596	1027	259	298	12			
1	R	210	Total	C	N	O	S	0	0	0
			1585	1014	259	300	12			
1	S	205	Total	C	N	O	S	0	0	0
			1533	978	254	290	11			
1	T	204	Total	C	N	O	S	0	0	0
			1541	987	249	293	12			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
A	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
A	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
A	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
A	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
A	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
A	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
A	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
B	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
B	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
C	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
C	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
C	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
C	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
C	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
C	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
C	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
D	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
D	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
D	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
D	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
D	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
D	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
E	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
E	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
E	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
E	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
E	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
E	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
F	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
F	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
F	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
F	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
F	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
F	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
G	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
G	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
G	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
G	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
G	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
H	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
H	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
H	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
H	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
H	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
H	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
I	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
I	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
I	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
I	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
I	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
I	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
J	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
J	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
J	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
J	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
J	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
J	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
J	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
J	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
J	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
J	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
J	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
K	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
K	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
K	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
K	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
K	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
K	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
L	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
L	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
L	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
L	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
L	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
L	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
M	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
M	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
M	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
M	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
M	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
M	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1

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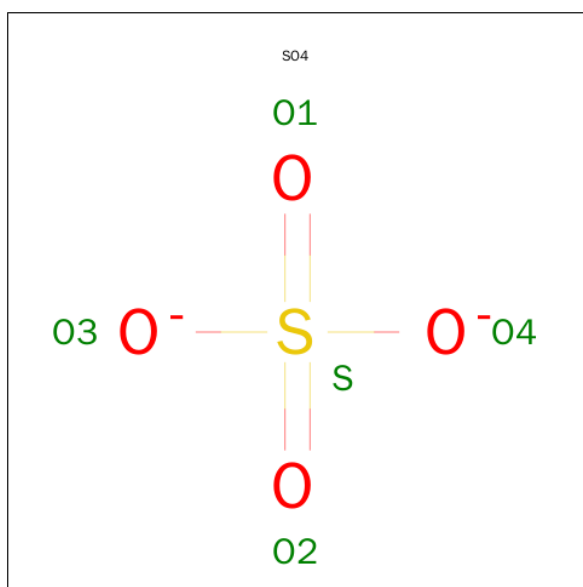
Chain	Residue	Modelled	Actual	Comment	Reference
N	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
N	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
N	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
N	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
N	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
N	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
O	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
O	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
O	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
O	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
O	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
O	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
P	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
P	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
P	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
P	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
P	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
P	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1

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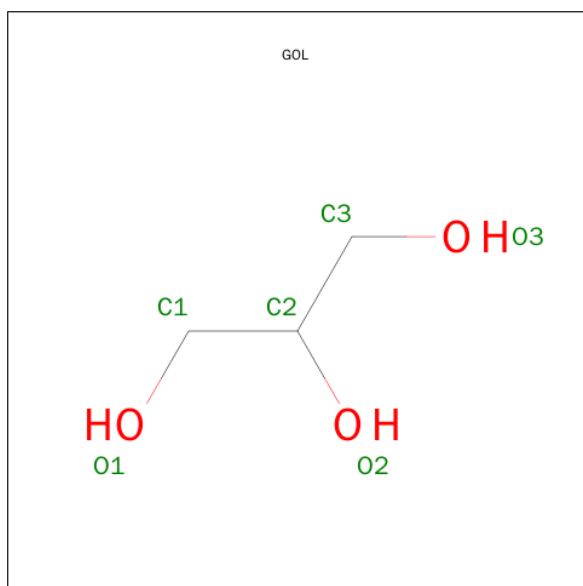
Chain	Residue	Modelled	Actual	Comment	Reference
Q	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
Q	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
R	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
R	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
R	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
R	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
R	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
R	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
S	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
S	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
S	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
S	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
S	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
S	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-11	MET	-	LEADER SEQUENCE	UNP Q9WYD1
T	-10	GLY	-	LEADER SEQUENCE	UNP Q9WYD1
T	-9	SER	-	LEADER SEQUENCE	UNP Q9WYD1
T	-8	ASP	-	LEADER SEQUENCE	UNP Q9WYD1
T	-7	LYS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-6	ILE	-	LEADER SEQUENCE	UNP Q9WYD1
T	-5	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-4	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-3	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-2	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	-1	HIS	-	LEADER SEQUENCE	UNP Q9WYD1
T	0	HIS	-	LEADER SEQUENCE	UNP Q9WYD1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	R	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	S	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	1
			10	5	5		
3	N	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		
3	Q	1	Total	C	O	0	0
			6	3	3		
3	T	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		

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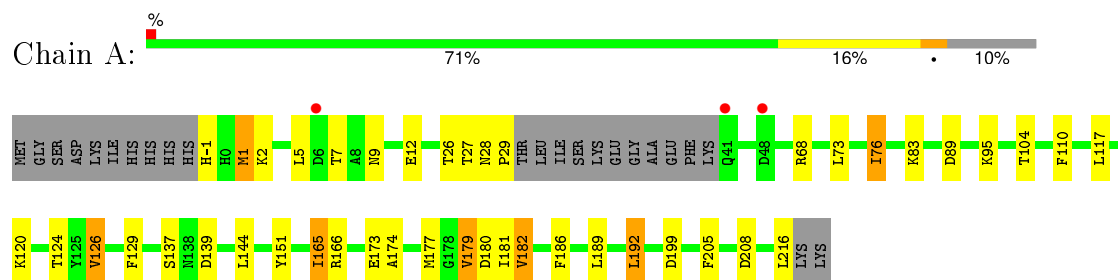
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	6	Total O 6 6	0	0
4	C	7	Total O 7 7	0	0
4	D	16	Total O 16 16	0	0
4	E	7	Total O 7 7	0	0
4	F	5	Total O 5 5	0	0
4	G	17	Total O 17 17	0	0
4	H	3	Total O 3 3	0	0
4	I	4	Total O 4 4	0	0
4	J	7	Total O 7 7	0	0
4	K	3	Total O 3 3	0	0
4	L	1	Total O 1 1	0	0
4	M	2	Total O 2 2	0	0
4	O	5	Total O 5 5	0	0
4	P	3	Total O 3 3	0	0
4	Q	7	Total O 7 7	0	0
4	R	2	Total O 2 2	0	0
4	S	2	Total O 2 2	0	0
4	T	1	Total O 1 1	0	0

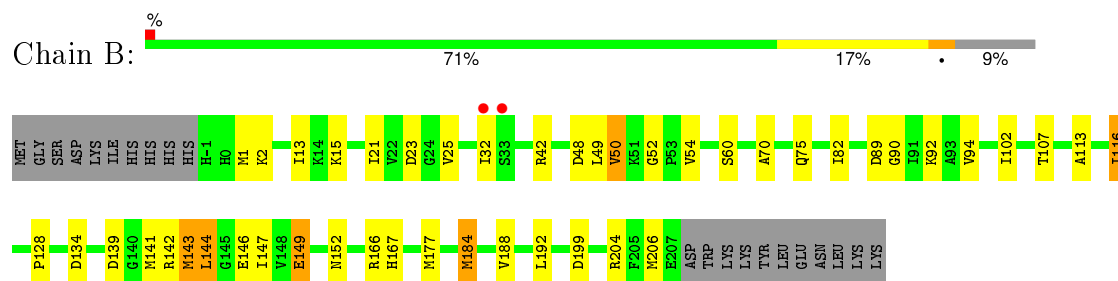
### 3 Residue-property plots [i](#)

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.

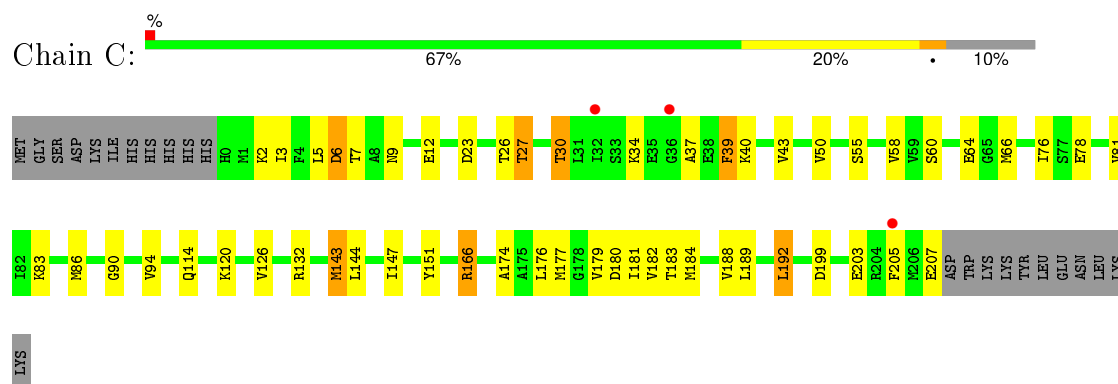
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

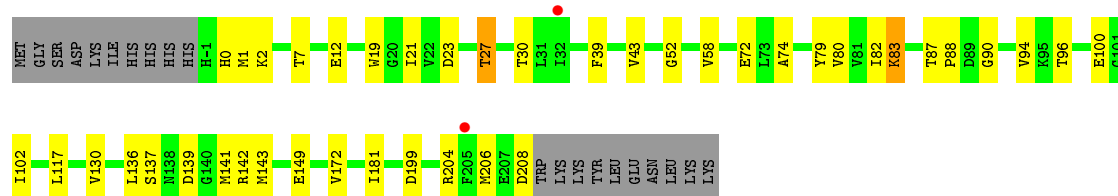


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



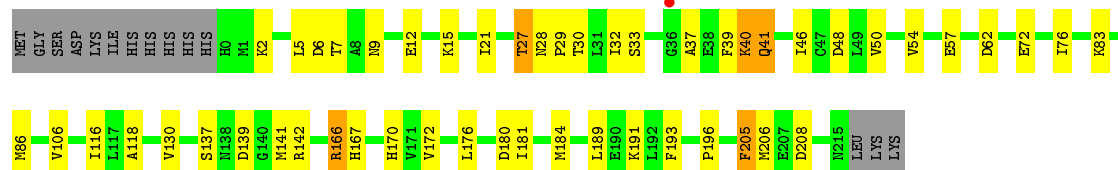
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))





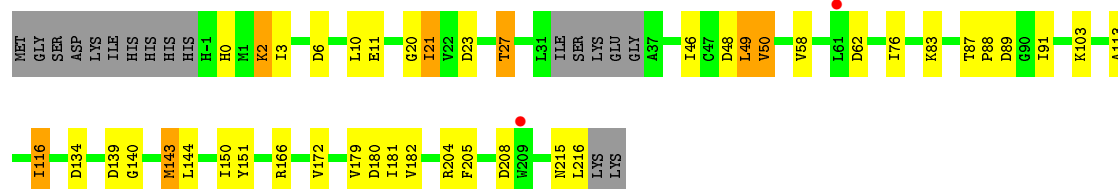
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain E: 72% 20% 6%



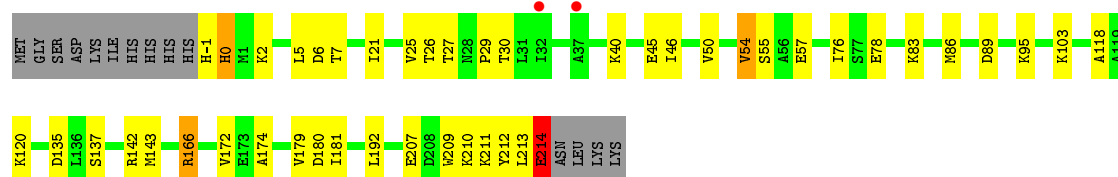
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain F: 74% 16% 7%



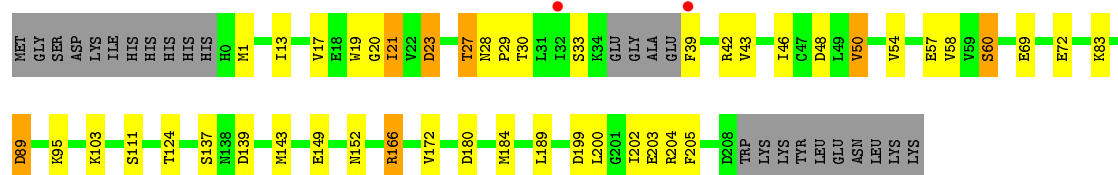
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

Chain G: 74% 18% 6%

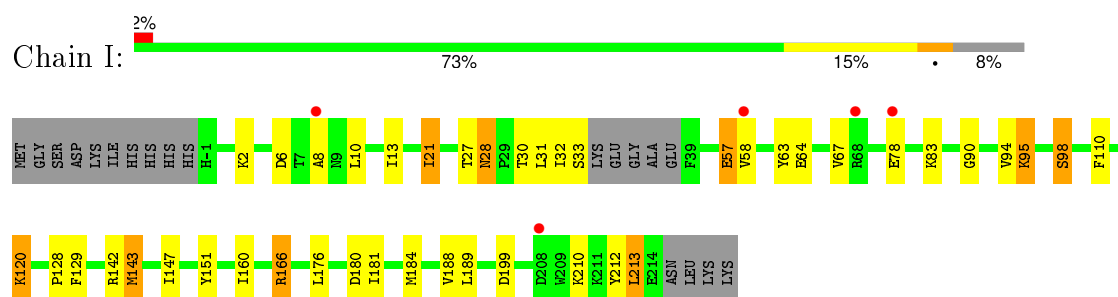


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

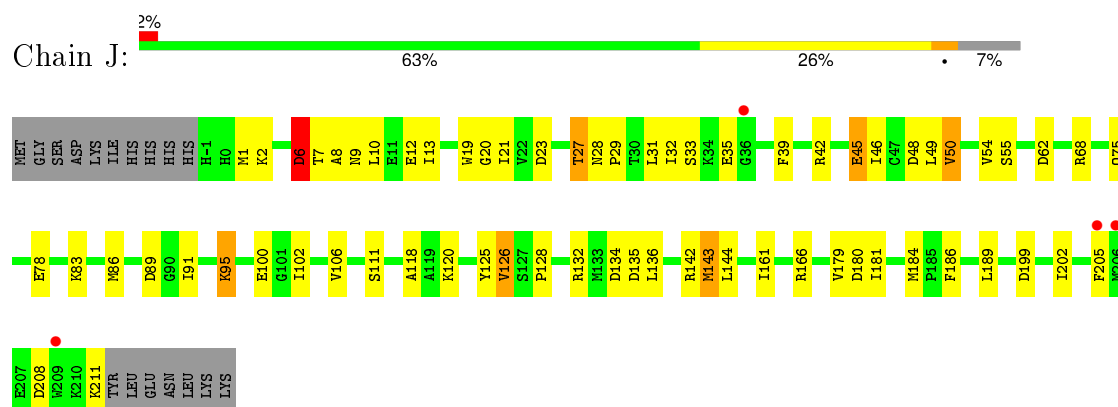
Chain H: 69% 17% 11%



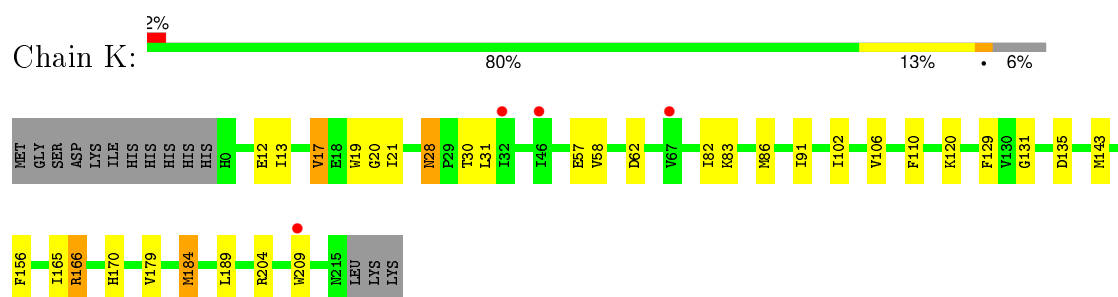
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



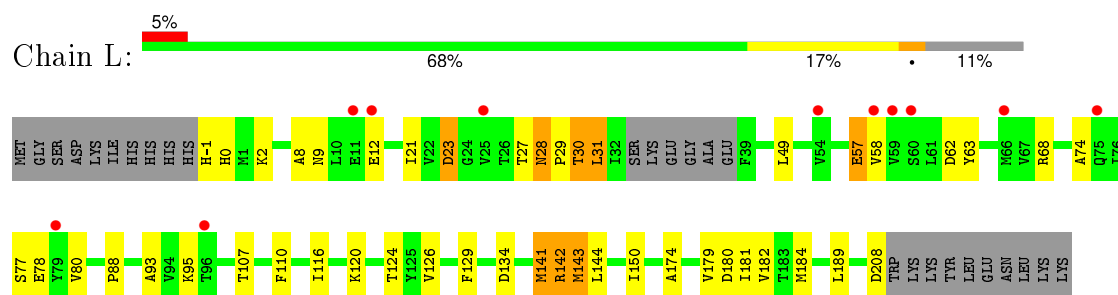
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



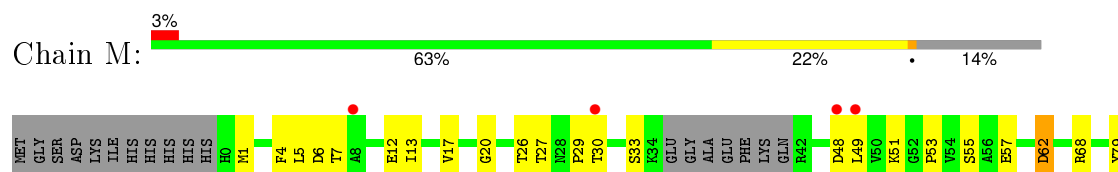
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



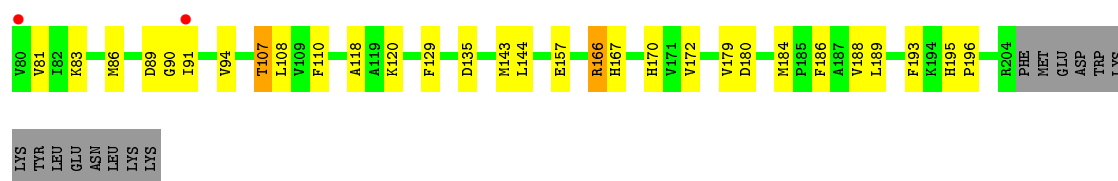
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



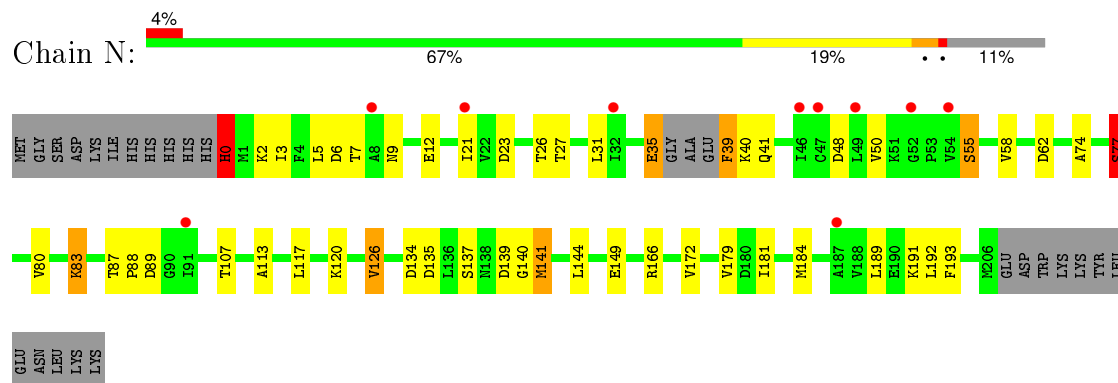
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



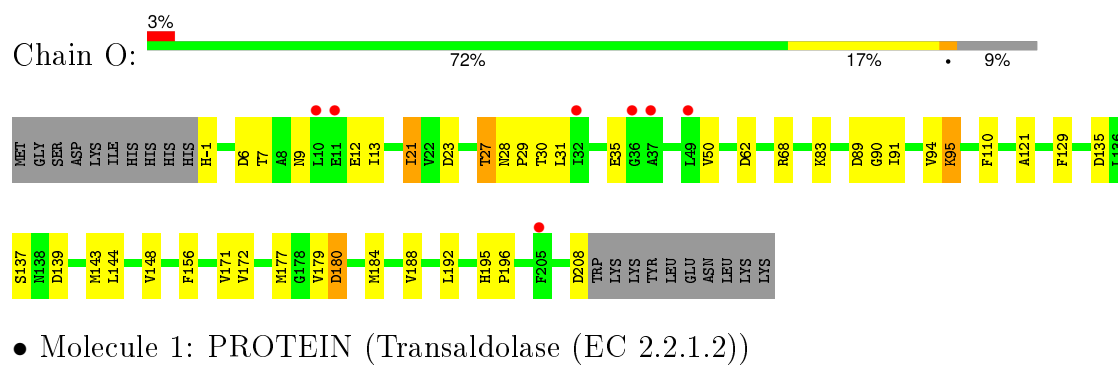




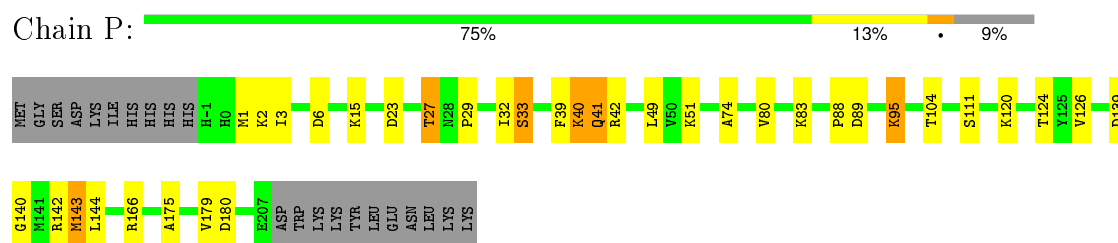
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



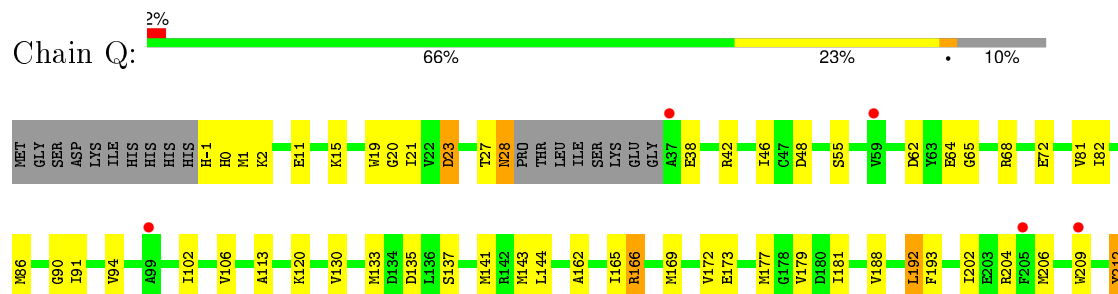
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

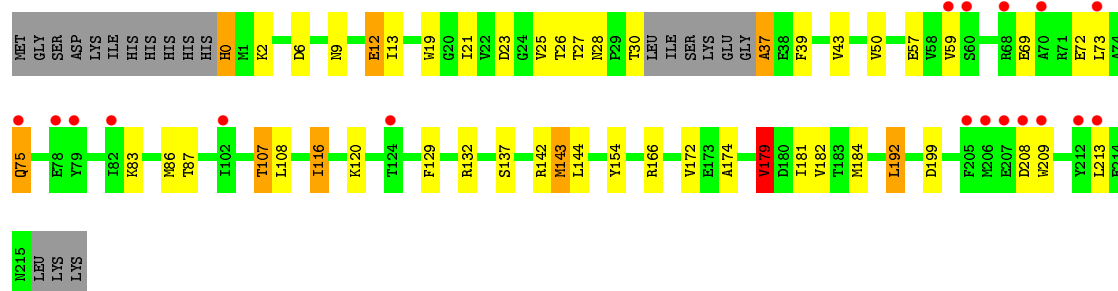


- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))

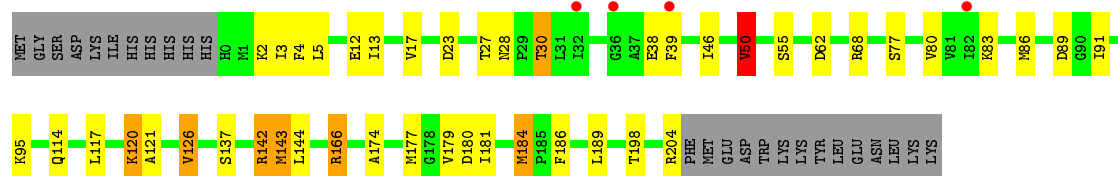




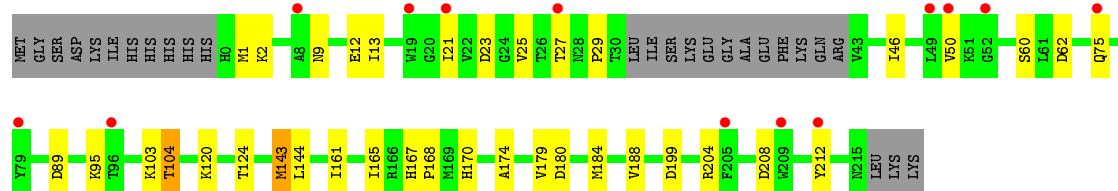
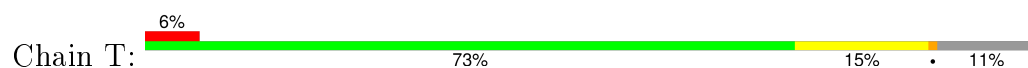
- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



- Molecule 1: PROTEIN (Transaldolase (EC 2.2.1.2))



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.30Å 104.42Å 171.12Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	83.13 – 2.40 83.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	85.9 (83.13-2.40) 85.5 (83.13-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.247 0.204 , 0.250	Depositor DCC
$R_{free}$ test set	8140 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 162006 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	31916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: GOL, SO4

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	0.72	0/1620	0.89	5/2194 (0.2%)
1	B	0.74	0/1612	0.85	5/2182 (0.2%)
1	C	0.77	1/1586 (0.1%)	0.87	6/2147 (0.3%)
1	D	0.84	0/1643	0.88	3/2223 (0.1%)
1	E	0.83	0/1704	0.91	7/2305 (0.3%)
1	F	0.76	0/1685	0.94	9/2280 (0.4%)
1	G	1.05	2/1698 (0.1%)	0.96	6/2300 (0.3%)
1	H	0.74	0/1576	0.90	8/2136 (0.4%)
1	I	0.85	3/1643 (0.2%)	0.90	5/2226 (0.2%)
1	J	1.33	4/1649 (0.2%)	0.94	10/2236 (0.4%)
1	K	0.68	0/1681	0.80	1/2279 (0.0%)
1	L	0.60	0/1556	0.83	4/2111 (0.2%)
1	M	0.59	0/1481	0.79	6/2009 (0.3%)
1	N	1.17	11/1498 (0.7%)	0.93	14/2027 (0.7%)
1	O	0.77	0/1632	0.86	5/2209 (0.2%)
1	P	0.69	0/1603	0.88	5/2172 (0.2%)
1	Q	0.75	3/1625 (0.2%)	0.85	6/2200 (0.3%)
1	R	0.70	3/1613 (0.2%)	0.84	4/2188 (0.2%)
1	S	0.63	0/1559	0.85	5/2112 (0.2%)
1	T	0.61	0/1569	0.78	3/2128 (0.1%)
All	All	0.81	27/32233 (0.1%)	0.88	117/43664 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1
1	N	0	1
1	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	45	GLU	CD-OE2	31.92	1.60	1.25
1	J	45	GLU	CD-OE1	28.67	1.57	1.25
1	G	214	GLU	C-O	23.22	1.67	1.23
1	N	35	GLU	CD-OE1	19.15	1.46	1.25
1	N	39	PHE	N-CA	15.11	1.76	1.46
1	N	39	PHE	C-O	14.94	1.51	1.23
1	N	35	GLU	CD-OE2	10.81	1.37	1.25
1	R	37	ALA	C-O	10.78	1.43	1.23
1	N	41	GLN	C-O	10.53	1.43	1.23
1	N	41	GLN	C-N	10.07	1.57	1.34
1	N	77	SER	CB-OG	9.64	1.54	1.42
1	Q	38	GLU	CD-OE2	9.64	1.36	1.25
1	Q	38	GLU	CD-OE1	8.95	1.35	1.25
1	N	40	LYS	C-O	8.43	1.39	1.23
1	J	211	LYS	C-O	8.10	1.38	1.23
1	I	64	GLU	CD-OE1	6.71	1.33	1.25
1	C	37	ALA	C-O	6.66	1.36	1.23
1	N	40	LYS	C-N	6.58	1.49	1.34
1	N	41	GLN	CA-C	6.15	1.69	1.52
1	I	33	SER	C-O	5.78	1.34	1.23
1	I	151	TYR	CD1-CE1	5.60	1.47	1.39
1	R	37	ALA	C-N	5.42	1.46	1.34
1	N	39	PHE	C-N	5.33	1.46	1.34
1	Q	28	ASN	CB-CG	5.27	1.63	1.51
1	G	45	GLU	CG-CD	5.17	1.59	1.51
1	J	45	GLU	CG-CD	5.14	1.59	1.51
1	R	57	GLU	CG-CD	5.04	1.59	1.51

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	166	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	G	166	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	G	214	GLU	CA-C-O	-8.57	102.11	120.10
1	P	89	ASP	CB-CG-OD2	7.95	125.45	118.30
1	F	48	ASP	CB-CG-OD2	7.90	125.41	118.30
1	N	41	GLN	CA-C-N	-7.67	100.32	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	ASP	CB-CG-OD2	7.50	125.05	118.30
1	J	89	ASP	CB-CG-OD2	7.31	124.88	118.30
1	F	62	ASP	CB-CG-OD2	7.24	124.82	118.30
1	J	62	ASP	CB-CG-OD2	7.22	124.80	118.30
1	H	89	ASP	CB-CG-OD2	7.18	124.77	118.30
1	H	180	ASP	CB-CG-OD2	7.09	124.68	118.30
1	F	23	ASP	CB-CG-OD2	7.08	124.67	118.30
1	R	6	ASP	CB-CG-OD2	7.00	124.60	118.30
1	C	23	ASP	CB-CG-OD2	6.77	124.39	118.30
1	P	23	ASP	CB-CG-OD2	6.76	124.39	118.30
1	O	180	ASP	CB-CG-OD2	6.67	124.30	118.30
1	J	134	ASP	CB-CG-OD1	6.65	124.29	118.30
1	C	166	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	G	180	ASP	CB-CG-OD2	6.55	124.19	118.30
1	N	89	ASP	CB-CG-OD2	6.55	124.19	118.30
1	G	6	ASP	CB-CG-OD2	6.53	124.18	118.30
1	F	208	ASP	CB-CG-OD2	6.49	124.14	118.30
1	Q	23	ASP	CB-CG-OD2	6.46	124.11	118.30
1	F	134	ASP	CB-CG-OD2	6.45	124.11	118.30
1	L	62	ASP	CB-CG-OD1	6.42	124.08	118.30
1	M	180	ASP	CB-CG-OD2	6.42	124.07	118.30
1	H	48	ASP	CB-CG-OD2	6.40	124.06	118.30
1	H	166	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	J	180	ASP	CB-CG-OD2	6.38	124.04	118.30
1	I	180	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	199	ASP	CB-CG-OD2	6.32	123.98	118.30
1	J	6	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	89	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	208	ASP	CB-CG-OD2	6.26	123.94	118.30
1	S	180	ASP	CB-CG-OD2	6.26	123.94	118.30
1	E	139	ASP	CB-CG-OD2	6.25	123.92	118.30
1	N	6	ASP	CB-CG-OD2	6.24	123.92	118.30
1	N	35	GLU	OE1-CD-OE2	6.22	130.76	123.30
1	N	39	PHE	CA-C-O	6.20	133.13	120.10
1	I	199	ASP	CB-CG-OD2	6.20	123.88	118.30
1	H	199	ASP	CB-CG-OD2	6.17	123.86	118.30
1	M	48	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	139	ASP	CB-CG-OD2	6.14	123.83	118.30
1	F	139	ASP	CB-CG-OD2	6.10	123.79	118.30
1	O	89	ASP	CB-CG-OD2	6.09	123.79	118.30
1	J	48	ASP	CB-CG-OD2	6.08	123.77	118.30
1	J	208	ASP	CB-CG-OD1	6.04	123.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	166	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	180	ASP	CB-CG-OD2	5.99	123.69	118.30
1	J	45	GLU	OE1-CD-OE2	5.98	130.48	123.30
1	O	62	ASP	CB-CG-OD2	5.96	123.67	118.30
1	S	126	VAL	CB-CA-C	-5.93	100.13	111.40
1	P	180	ASP	CB-CG-OD2	5.92	123.63	118.30
1	L	180	ASP	CB-CG-OD2	5.90	123.61	118.30
1	L	23	ASP	CB-CG-OD2	5.90	123.61	118.30
1	P	139	ASP	CB-CG-OD2	5.81	123.53	118.30
1	S	62	ASP	CB-CG-OD2	5.77	123.49	118.30
1	N	48	ASP	CB-CG-OD2	5.72	123.45	118.30
1	R	199	ASP	CB-CG-OD2	5.72	123.45	118.30
1	K	62	ASP	CB-CG-OD2	5.69	123.42	118.30
1	D	199	ASP	CB-CG-OD2	5.68	123.41	118.30
1	M	6	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	139	ASP	CB-CG-OD2	5.64	123.38	118.30
1	I	6	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	199	ASP	CB-CG-OD2	5.63	123.36	118.30
1	Q	166	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	180	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	89	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	166	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	P	6	ASP	CB-CG-OD2	5.53	123.28	118.30
1	I	166	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	R	179	VAL	CB-CA-C	-5.51	100.94	111.40
1	F	6	ASP	CB-CG-OD2	5.47	123.22	118.30
1	N	126	VAL	CB-CA-C	-5.45	101.05	111.40
1	E	62	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	48	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	208	ASP	CB-CG-OD2	5.38	123.14	118.30
1	T	199	ASP	CB-CG-OD2	5.36	123.12	118.30
1	S	166	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	S	50	VAL	CB-CA-C	-5.35	101.24	111.40
1	E	208	ASP	CB-CG-OD2	5.33	123.10	118.30
1	N	139	ASP	CB-CG-OD2	5.33	123.09	118.30
1	H	23	ASP	CB-CG-OD2	5.28	123.05	118.30
1	N	0	HIS	N-CA-CB	-5.27	101.11	110.60
1	B	134	ASP	CB-CG-OD1	5.26	123.03	118.30
1	T	180	ASP	CB-CG-OD2	5.23	123.01	118.30
1	H	139	ASP	CB-CG-OD2	5.23	123.00	118.30
1	L	142	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	N	23	ASP	CB-CG-OD2	5.21	122.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	VAL	CB-CA-C	-5.21	101.50	111.40
1	M	89	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	199	ASP	CB-CG-OD2	5.20	122.98	118.30
1	O	135	ASP	CB-CA-C	-5.19	100.01	110.40
1	R	208	ASP	CB-CG-OD2	5.16	122.94	118.30
1	M	62	ASP	CB-CG-OD2	5.15	122.93	118.30
1	H	50	VAL	CB-CA-C	-5.15	101.62	111.40
1	N	62	ASP	CB-CG-OD2	5.15	122.93	118.30
1	F	89	ASP	CB-CG-OD2	5.14	122.93	118.30
1	C	6	ASP	CB-CG-OD2	5.13	122.92	118.30
1	I	21	ILE	CB-CA-C	-5.12	101.36	111.60
1	N	41	GLN	C-N-CA	-5.12	108.90	121.70
1	C	166	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	Q	177	MET	CB-CA-C	-5.12	100.17	110.40
1	T	89	ASP	CB-CG-OD2	5.11	122.90	118.30
1	M	135	ASP	CB-CG-OD2	5.10	122.89	118.30
1	N	135	ASP	CB-CG-OD2	5.10	122.89	118.30
1	Q	62	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	135	ASP	CB-CG-OD2	5.07	122.87	118.30
1	Q	48	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	180	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	48	ASP	CB-CG-OD2	5.05	122.85	118.30
1	N	39	PHE	CA-C-N	-5.05	106.09	117.20
1	G	89	ASP	CB-CG-OD2	5.03	122.83	118.30
1	E	166	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	O	139	ASP	CB-CG-OD2	5.02	122.82	118.30
1	J	126	VAL	CB-CA-C	-5.02	101.87	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	-1	HIS	Peptide
1	N	35	GLU	Sidechain
1	R	37	ALA	Mainchain

## 5.2 Too-close contacts ⓘ

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



the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1591	0	1601	32	0
1	B	1584	0	1598	31	0
1	C	1560	0	1561	32	0
1	D	1615	0	1642	29	0
1	E	1674	0	1703	35	0
1	F	1655	0	1680	18	0
1	G	1667	0	1680	27	0
1	H	1550	0	1557	28	0
1	I	1615	0	1623	29	0
1	J	1619	0	1617	51	0
1	K	1651	0	1648	23	0
1	L	1530	0	1521	27	0
1	M	1457	0	1439	32	0
1	N	1475	0	1446	29	0
1	O	1604	0	1613	30	0
1	P	1576	0	1590	21	0
1	Q	1596	0	1594	32	0
1	R	1585	0	1569	28	0
1	S	1533	0	1538	27	0
1	T	1541	0	1521	19	0
2	O	5	0	0	0	0
3	A	6	0	8	1	0
3	B	6	0	8	1	0
3	C	6	0	8	1	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	1	0
3	G	6	0	8	0	0
3	H	6	0	8	2	0
3	I	6	0	8	0	0
3	J	6	0	8	0	0
3	K	10	0	16	0	0
3	L	6	0	8	0	0
3	M	6	0	8	0	0
3	N	6	0	8	0	0
3	O	6	0	8	3	0
3	P	12	0	16	1	0
3	Q	6	0	8	0	0
3	R	6	0	8	0	0
3	S	6	0	8	0	0
3	T	6	0	8	0	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	1	0
4	C	7	0	0	0	0
4	D	16	0	0	2	0
4	E	7	0	0	0	0
4	F	5	0	0	0	0
4	G	17	0	0	1	0
4	H	3	0	0	0	0
4	I	4	0	0	0	0
4	J	7	0	0	0	0
4	K	3	0	0	0	0
4	L	1	0	0	0	0
4	M	2	0	0	0	0
4	O	5	0	0	0	0
4	P	3	0	0	0	0
4	Q	7	0	0	0	0
4	R	2	0	0	0	0
4	S	2	0	0	0	0
4	T	1	0	0	0	0
All	All	31916	0	31917	496	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (496) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:39:PHE:CA	1:N:39:PHE:N	1.76	1.48
1:G:214:GLU:C	1:G:214:GLU:O	1.67	1.30
1:O:156:PHE:O	3:O:220:GOL:H31	1.63	0.96
1:L:142:ARG:CZ	1:S:142:ARG:HD2	2.10	0.80
1:K:184:MET:CE	1:K:189:LEU:HB2	2.12	0.79
1:J:28:ASN:CB	1:J:29:PRO:HD2	2.11	0.79
1:J:31:LEU:O	1:J:35:GLU:HG2	1.82	0.79
1:J:28:ASN:CG	1:J:29:PRO:HD2	2.04	0.78
1:M:184:MET:HE1	1:M:189:LEU:HA	1.66	0.78
1:D:7:THR:HG22	4:D:226:HOH:O	1.82	0.77
1:A:28:ASN:HB2	1:A:29:PRO:HD2	1.65	0.77
1:J:28:ASN:OD1	1:J:29:PRO:HD2	1.86	0.75
1:Q:120:LYS:NZ	1:R:23:ASP:OD2	2.20	0.74
1:D:74:ALA:HA	1:D:80:VAL:HG11	1.68	0.74
1:K:184:MET:HE1	1:K:189:LEU:HB2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:LYS:HG2	1:G:76:ILE:HD11	1.70	0.74
1:J:128:PRO:HB3	1:J:143:MET:CE	2.18	0.73
1:A:174:ALA:HB1	1:A:179:VAL:HG21	1.70	0.73
1:F:27:THR:O	1:F:83:LYS:NZ	2.20	0.73
1:N:27:THR:O	1:N:83:LYS:NZ	2.22	0.73
1:K:28:ASN:ND2	1:K:31:LEU:H	1.87	0.72
1:B:70:ALA:HB1	1:B:82:ILE:HD13	1.70	0.72
1:E:27:THR:O	1:E:83:LYS:NZ	2.22	0.72
1:G:27:THR:HG22	1:G:55:SER:O	1.90	0.71
1:L:184:MET:HE1	1:L:189:LEU:HA	1.72	0.71
1:N:144:LEU:HD21	1:N:179:VAL:HG21	1.73	0.71
1:J:8:ALA:HB3	1:J:35:GLU:HG3	1.73	0.70
1:P:40:LYS:O	1:P:41:GLN:HB2	1.90	0.70
1:S:77:SER:O	1:S:80:VAL:HG12	1.90	0.70
1:N:120:LYS:NZ	1:O:23:ASP:OD2	2.24	0.70
1:D:172:VAL:HG21	1:H:137:SER:HB2	1.72	0.70
1:J:128:PRO:HB3	1:J:143:MET:HE1	1.74	0.70
1:R:120:LYS:NZ	1:S:23:ASP:OD2	2.25	0.69
1:D:7:THR:HG21	1:D:12:GLU:OE1	1.92	0.69
1:A:27:THR:O	1:A:83:LYS:NZ	2.22	0.69
1:H:13:ILE:O	1:H:17:VAL:HG23	1.94	0.68
1:A:117:LEU:HD22	1:B:21:ILE:HD12	1.76	0.68
1:J:86:MET:HE1	1:J:118:ALA:HB2	1.74	0.68
1:D:27:THR:O	1:D:83:LYS:NZ	2.22	0.68
1:A:120:LYS:NZ	1:B:23:ASP:OD2	2.26	0.68
1:G:27:THR:O	1:G:83:LYS:NZ	2.26	0.67
1:H:202:ILE:O	1:H:205:PHE:HB3	1.95	0.67
1:E:184:MET:CE	1:E:189:LEU:HA	2.24	0.67
1:K:135:ASP:OD2	1:K:166:ARG:NH2	2.28	0.67
1:H:203:GLU:O	1:H:205:PHE:N	2.26	0.67
1:O:156:PHE:O	3:O:220:GOL:C3	2.39	0.66
1:K:184:MET:HE1	1:K:189:LEU:CB	2.25	0.66
1:Q:135:ASP:OD2	1:Q:166:ARG:NH2	2.28	0.66
1:N:77:SER:O	1:N:80:VAL:HG12	1.94	0.66
1:O:137:SER:HB3	1:Q:172:VAL:HG21	1.76	0.66
1:K:28:ASN:C	1:K:28:ASN:HD22	1.98	0.66
1:H:60:SER:HB2	1:H:69:GLU:OE2	1.95	0.66
1:N:184:MET:HE1	1:N:189:LEU:HA	1.78	0.65
1:H:203:GLU:C	1:H:205:PHE:H	2.00	0.65
1:A:73:LEU:HD23	1:A:76:ILE:HD11	1.78	0.65
1:I:95:LYS:HG3	1:J:20:GLY:HA3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:THR:O	1:H:83:LYS:NZ	2.25	0.65
1:M:144:LEU:HD21	1:M:179:VAL:HG21	1.79	0.64
1:L:110:PHE:CE1	1:L:129:PHE:HB2	2.33	0.64
1:S:120:LYS:HE3	1:T:1:MET:O	1.97	0.64
1:J:144:LEU:HD21	1:J:179:VAL:HG21	1.81	0.63
1:A:1:MET:HE1	1:E:116:ILE:HD13	1.81	0.63
1:E:21:ILE:HD12	1:E:189:LEU:HD11	1.82	0.62
1:P:120:LYS:NZ	1:Q:23:ASP:OD2	2.27	0.62
1:C:120:LYS:NZ	1:D:23:ASP:OD2	2.25	0.62
1:T:25:VAL:CG2	1:T:50:VAL:HG21	2.30	0.62
1:A:28:ASN:CB	1:A:29:PRO:HD2	2.30	0.61
1:M:12:GLU:OE1	1:M:186:PHE:HB2	2.00	0.61
1:E:137:SER:HB3	1:G:172:VAL:HG21	1.82	0.61
1:P:1:MET:O	1:T:120:LYS:NZ	2.29	0.61
1:A:26:THR:HG23	1:A:83:LYS:NZ	2.16	0.61
1:G:120:LYS:NZ	1:H:23:ASP:OD2	2.27	0.61
1:F:2:LYS:HB2	1:F:181:ILE:HG12	1.81	0.60
1:B:144:LEU:HD13	1:B:177:MET:HE1	1.83	0.60
1:A:174:ALA:HB1	1:A:179:VAL:CG2	2.31	0.60
1:N:0:HIS:H3	1:N:0:HIS:CD2	2.19	0.60
1:G:0:HIS:ND1	4:G:225:HOH:O	2.31	0.60
1:A:189:LEU:HA	1:A:192:LEU:HD22	1.84	0.60
1:R:39:PHE:O	1:R:43:VAL:HG23	2.01	0.59
1:C:90:GLY:O	1:C:94:VAL:HG23	2.02	0.59
1:B:116:ILE:HD11	1:C:3:ILE:HD11	1.84	0.59
1:A:144:LEU:HG	1:A:177:MET:HE1	1.84	0.59
1:J:9:ASN:HB3	1:J:12:GLU:HG2	1.83	0.59
1:P:1:MET:HE3	1:P:175:ALA:HA	1.84	0.59
1:O:28:ASN:CG	1:O:29:PRO:HD2	2.23	0.59
1:C:184:MET:HE1	1:C:189:LEU:HA	1.83	0.59
1:L:77:SER:O	1:L:80:VAL:HG12	2.02	0.59
1:T:184:MET:CE	1:T:188:VAL:HG12	2.33	0.59
1:J:27:THR:HG23	1:J:32:ILE:HD11	1.83	0.59
1:N:0:HIS:N	1:N:0:HIS:CD2	2.66	0.59
1:I:57:GLU:HA	1:I:83:LYS:HB2	1.85	0.59
1:Q:-1:HIS:CG	1:Q:0:HIS:H	2.20	0.59
1:Q:169:MET:O	1:Q:173:GLU:HG3	2.02	0.59
1:A:26:THR:HG23	1:A:83:LYS:HZ2	1.68	0.59
1:D:137:SER:HB2	1:H:172:VAL:HG21	1.85	0.59
1:P:74:ALA:HA	1:P:80:VAL:CG1	2.31	0.58
1:M:107:THR:HG23	1:M:108:LEU:HG	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ASN:OD1	3:H:219:GOL:H31	2.03	0.58
1:N:39:PHE:N	1:N:39:PHE:C	2.56	0.58
1:R:28:ASN:OD1	1:R:30:THR:OG1	2.20	0.58
1:D:117:LEU:HD22	1:E:21:ILE:HD13	1.85	0.58
1:F:151:TYR:HB3	3:F:219:GOL:H31	1.85	0.58
1:K:86:MET:HE2	1:K:106:VAL:HG11	1.84	0.58
1:K:28:ASN:HD21	1:K:31:LEU:H	1.51	0.57
1:A:73:LEU:O	1:A:76:ILE:HG13	2.03	0.57
1:J:184:MET:HE2	1:J:189:LEU:HB2	1.85	0.57
1:F:116:ILE:CG2	1:F:150:ILE:HG21	2.33	0.57
1:N:74:ALA:HA	1:N:80:VAL:HG11	1.85	0.57
1:J:19:TRP:HB3	1:J:21:ILE:HD12	1.86	0.57
1:P:74:ALA:HA	1:P:80:VAL:HG11	1.86	0.57
1:C:151:TYR:HB3	3:C:219:GOL:H31	1.85	0.57
1:J:28:ASN:CB	1:J:29:PRO:CD	2.81	0.57
1:L:74:ALA:HA	1:L:80:VAL:HG11	1.87	0.57
1:B:142:ARG:HD3	1:I:142:ARG:CZ	2.35	0.57
1:A:9:ASN:HB3	1:A:12:GLU:HG2	1.87	0.57
1:C:120:LYS:HE3	1:D:1:MET:O	2.04	0.57
1:J:184:MET:CE	1:J:189:LEU:HA	2.35	0.57
1:B:142:ARG:HD3	1:I:142:ARG:NE	2.19	0.57
1:L:120:LYS:HE3	1:M:1:MET:O	2.03	0.57
1:L:95:LYS:HG3	1:M:20:GLY:HA3	1.87	0.57
1:O:9:ASN:HB3	1:O:12:GLU:CG	2.34	0.57
1:M:90:GLY:O	1:M:94:VAL:HG23	2.04	0.57
1:A:137:SER:HB2	1:F:172:VAL:HG21	1.87	0.57
1:A:174:ALA:O	1:A:179:VAL:HG23	2.05	0.57
1:C:40:LYS:HG2	1:C:76:ILE:HD11	1.86	0.57
1:M:184:MET:HE3	1:M:188:VAL:HG12	1.86	0.56
1:N:172:VAL:HG21	1:R:137:SER:HB3	1.87	0.56
1:P:27:THR:O	1:P:83:LYS:NZ	2.26	0.56
1:C:184:MET:HE1	1:C:189:LEU:CA	2.34	0.56
1:P:51:LYS:O	3:P:220:GOL:H11	2.05	0.56
1:G:29:PRO:HD3	1:G:57:GLU:CD	2.26	0.56
1:A:12:GLU:HB2	1:A:186:PHE:CD1	2.41	0.56
1:N:137:SER:HB2	1:R:172:VAL:HG21	1.88	0.56
1:R:116:ILE:HD11	1:S:3:ILE:HD11	1.87	0.56
1:C:5:LEU:HB3	1:C:7:THR:HG22	1.88	0.56
1:M:172:VAL:HG21	1:S:137:SER:HB3	1.87	0.56
1:S:184:MET:CE	1:S:189:LEU:HA	2.37	0.56
1:M:184:MET:HE1	1:M:189:LEU:CA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:172:VAL:HG21	1:Q:137:SER:OG	2.06	0.55
1:C:58:VAL:HG21	1:C:66:MET:HG2	1.87	0.55
1:F:116:ILE:HG21	1:F:150:ILE:HG21	1.88	0.55
1:R:25:VAL:HG23	1:R:50:VAL:HG21	1.88	0.55
1:R:26:THR:HB	1:R:83:LYS:HZ1	1.70	0.55
1:F:144:LEU:HD21	1:F:179:VAL:HG21	1.87	0.55
1:N:141:MET:HA	1:N:141:MET:HE2	1.89	0.55
1:E:46:ILE:O	1:E:50:VAL:HG12	2.07	0.55
1:R:19:TRP:HB3	1:R:21:ILE:HD12	1.87	0.55
1:A:110:PHE:CE1	1:A:129:PHE:HB2	2.41	0.55
1:E:9:ASN:HB3	1:E:12:GLU:HG2	1.88	0.55
1:E:191:LYS:NZ	1:G:135:ASP:OD2	2.39	0.54
1:O:184:MET:HE3	1:O:188:VAL:HG12	1.88	0.54
1:G:86:MET:HE1	1:G:118:ALA:HB2	1.89	0.54
1:M:120:LYS:HZ3	1:N:3:ILE:HD12	1.72	0.54
1:M:13:ILE:O	1:M:17:VAL:HG23	2.07	0.54
1:G:214:GLU:CA	1:G:214:GLU:O	2.54	0.54
1:D:39:PHE:O	1:D:43:VAL:HG23	2.07	0.54
1:E:184:MET:HE2	1:E:189:LEU:HB2	1.88	0.54
1:M:166:ARG:H	1:M:170:HIS:HD2	1.56	0.54
1:N:26:THR:HG22	1:N:55:SER:OG	2.07	0.54
1:L:141:MET:CE	1:L:144:LEU:HD23	2.38	0.54
1:M:91:ILE:HD12	1:N:193:PHE:CE2	2.42	0.54
1:R:26:THR:HB	1:R:83:LYS:NZ	2.23	0.54
1:H:184:MET:CE	1:H:189:LEU:HA	2.37	0.54
1:N:117:LEU:HD22	1:O:21:ILE:CD1	2.38	0.54
1:E:86:MET:HE2	1:E:106:VAL:HG11	1.88	0.54
1:E:184:MET:HE2	1:E:189:LEU:CA	2.38	0.54
1:E:2:LYS:HB2	1:E:181:ILE:HG23	1.90	0.54
1:J:184:MET:HE1	1:J:189:LEU:HA	1.90	0.53
1:A:139:ASP:HB3	1:J:142:ARG:NH2	2.23	0.53
1:C:143:MET:CE	1:C:147:ILE:HD12	2.37	0.53
1:C:30:THR:O	1:C:34:LYS:HB2	2.08	0.53
1:R:0:HIS:ND1	1:R:0:HIS:N	2.54	0.53
1:D:74:ALA:HA	1:D:80:VAL:CG1	2.36	0.53
1:J:12:GLU:HB2	1:J:186:PHE:CD1	2.43	0.53
1:E:40:LYS:HB3	1:E:76:ILE:HD11	1.90	0.53
1:J:184:MET:CE	1:J:189:LEU:CA	2.87	0.53
1:L:28:ASN:ND2	1:L:30:THR:OG1	2.41	0.53
1:E:40:LYS:O	1:E:41:GLN:CB	2.57	0.53
1:H:39:PHE:O	1:H:43:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:MET:CE	1:E:189:LEU:CA	2.87	0.53
1:S:91:ILE:HG23	1:S:121:ALA:HB2	1.90	0.53
1:M:120:LYS:NZ	1:N:3:ILE:HD12	2.24	0.53
1:R:143:MET:HG3	1:R:144:LEU:N	2.23	0.53
1:G:46:ILE:O	1:G:50:VAL:HG12	2.09	0.53
1:J:28:ASN:O	1:J:32:ILE:N	2.38	0.52
1:A:173:GLU:O	1:A:177:MET:HG3	2.08	0.52
1:C:86:MET:HE3	1:C:114:GLN:HB3	1.90	0.52
1:B:152:ASN:OD1	3:B:219:GOL:O3	2.27	0.52
1:B:142:ARG:HD3	1:I:142:ARG:HD2	1.90	0.52
1:I:120:LYS:HE3	1:J:1:MET:O	2.09	0.52
1:J:86:MET:CE	1:J:106:VAL:HG11	2.40	0.52
1:J:9:ASN:HB3	1:J:12:GLU:CG	2.38	0.52
1:L:74:ALA:HA	1:L:80:VAL:CG1	2.39	0.52
1:M:29:PRO:HD2	1:M:57:GLU:OE2	2.09	0.52
1:H:46:ILE:HG22	1:H:54:VAL:HG21	1.91	0.52
1:A:137:SER:OG	1:J:111:SER:HB2	2.10	0.52
1:D:88:PRO:HA	1:E:193:PHE:CE2	2.44	0.52
1:D:142:ARG:HG2	1:G:142:ARG:CZ	2.40	0.52
1:D:149:GLU:HG2	1:E:176:LEU:HD23	1.92	0.52
1:F:216:LEU:O	1:F:216:LEU:HD12	2.09	0.52
1:F:205:PHE:CD1	1:J:29:PRO:HG2	2.45	0.52
1:G:120:LYS:HE3	1:H:1:MET:O	2.10	0.52
1:F:87:THR:HB	1:F:88:PRO:HD2	1.92	0.52
1:J:13:ILE:HG21	1:J:50:VAL:HG22	1.92	0.52
1:H:203:GLU:C	1:H:205:PHE:N	2.62	0.52
1:P:120:LYS:NZ	1:Q:1:MET:O	2.43	0.51
1:M:86:MET:SD	1:M:91:ILE:HD11	2.51	0.51
1:C:143:MET:CE	1:C:147:ILE:CD1	2.88	0.51
1:Q:133:MET:HG3	1:Q:143:MET:CE	2.39	0.51
1:K:120:LYS:NZ	1:L:23:ASP:OD2	2.29	0.51
1:B:142:ARG:HD3	1:I:142:ARG:CD	2.39	0.51
1:O:184:MET:CE	1:O:188:VAL:HG12	2.40	0.51
1:J:132:ARG:O	1:J:136:LEU:HD13	2.11	0.51
1:J:32:ILE:HD13	1:J:39:PHE:CD1	2.45	0.51
1:B:144:LEU:HD13	1:B:177:MET:CE	2.40	0.51
1:H:184:MET:HE2	1:H:189:LEU:HB2	1.92	0.51
1:G:5:LEU:HB3	1:G:7:THR:HG22	1.92	0.51
1:J:27:THR:CG2	1:J:32:ILE:HD11	2.40	0.51
1:Q:162:ALA:HB1	1:Q:165:ILE:HD11	1.92	0.51
1:G:211:LYS:O	1:G:214:GLU:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:86:MET:HE2	1:Q:106:VAL:HG11	1.91	0.51
1:G:174:ALA:HB1	1:G:179:VAL:HG11	1.93	0.51
1:I:21:ILE:HG22	1:I:21:ILE:O	2.11	0.51
1:S:28:ASN:OD1	1:S:30:THR:OG1	2.23	0.51
1:S:46:ILE:O	1:S:50:VAL:HG23	2.10	0.51
1:A:73:LEU:CD2	1:A:76:ILE:HD11	2.40	0.50
1:I:120:LYS:NZ	1:J:23:ASP:OD2	2.37	0.50
1:L:184:MET:HE1	1:L:189:LEU:CA	2.40	0.50
1:F:91:ILE:HG21	1:G:21:ILE:CD1	2.41	0.50
1:Q:144:LEU:HD21	1:Q:179:VAL:HG21	1.92	0.50
1:A:5:LEU:HB3	1:A:7:THR:HG22	1.92	0.50
1:T:13:ILE:CD1	1:T:46:ILE:HG23	2.42	0.50
1:R:184:MET:HE1	1:R:192:LEU:HD22	1.94	0.50
1:L:8:ALA:HB3	1:L:31:LEU:O	2.11	0.50
1:I:2:LYS:HB2	1:I:181:ILE:HG12	1.94	0.50
1:B:143:MET:HE3	1:B:147:ILE:HD11	1.94	0.50
1:A:2:LYS:HB2	1:A:181:ILE:HG12	1.93	0.50
1:N:74:ALA:HA	1:N:80:VAL:CG1	2.42	0.50
1:E:46:ILE:HG22	1:E:54:VAL:HG21	1.93	0.50
1:Q:42:ARG:O	1:Q:46:ILE:HG13	2.12	0.50
1:T:25:VAL:HG23	1:T:50:VAL:HG21	1.93	0.49
1:Q:65:GLY:HA2	1:Q:68:ARG:NH2	2.28	0.49
1:I:143:MET:CE	1:I:147:ILE:HD12	2.40	0.49
1:T:9:ASN:HB3	1:T:12:GLU:HG2	1.92	0.49
1:F:46:ILE:O	1:F:50:VAL:HG22	2.12	0.49
1:R:107:THR:HG23	1:R:108:LEU:HG	1.94	0.49
1:R:129:PHE:HD2	1:R:132:ARG:HD2	1.78	0.49
1:M:26:THR:HG22	1:M:83:LYS:HE2	1.94	0.49
1:M:184:MET:CE	1:M:189:LEU:N	2.75	0.49
1:A:104:THR:O	1:A:124:THR:HB	2.13	0.49
1:N:2:LYS:HB2	1:N:181:ILE:HG12	1.93	0.49
1:L:141:MET:HE3	1:L:144:LEU:HD23	1.93	0.49
1:K:13:ILE:O	1:K:17:VAL:HG13	2.13	0.49
1:S:120:LYS:NZ	1:T:23:ASP:OD2	2.43	0.49
1:D:130:VAL:HG11	1:D:141:MET:HE2	1.93	0.49
1:D:130:VAL:HG11	1:D:141:MET:CE	2.43	0.49
1:B:32:ILE:HG23	1:B:42:ARG:HG2	1.94	0.49
1:G:95:LYS:NZ	1:H:20:GLY:HA2	2.28	0.48
1:L:2:LYS:HB2	1:L:181:ILE:HG12	1.95	0.48
1:R:2:LYS:HB2	1:R:181:ILE:HG23	1.94	0.48
1:L:174:ALA:HB1	1:L:179:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:ILE:HD13	1:D:102:ILE:CG2	2.43	0.48
1:E:57:GLU:OE2	1:E:83:LYS:NZ	2.44	0.48
1:B:143:MET:CE	1:B:147:ILE:CD1	2.91	0.48
1:C:26:THR:HG22	1:C:55:SER:OG	2.13	0.48
1:S:184:MET:HE1	1:S:189:LEU:HA	1.95	0.48
1:J:202:ILE:O	1:J:205:PHE:HB3	2.13	0.48
1:C:177:MET:HE2	1:C:177:MET:HB2	1.67	0.48
1:M:157:GLU:CD	1:M:157:GLU:H	2.17	0.48
1:L:95:LYS:CG	1:M:20:GLY:HA3	2.44	0.48
1:Q:11:GLU:O	1:Q:15[B]:LYS:HG3	2.13	0.48
1:O:195:HIS:ND1	1:O:196:PRO:HD2	2.29	0.48
1:B:13:ILE:HG22	1:B:49:LEU:HG	1.96	0.48
1:Q:90:GLY:O	1:Q:94:VAL:HG23	2.14	0.48
1:H:103:LYS:HG2	1:H:124:THR:HG21	1.96	0.47
1:L:142:ARG:NH1	1:S:142:ARG:HH11	2.12	0.47
1:J:7:THR:HG21	1:J:12:GLU:OE2	2.14	0.47
1:E:196:PRO:HB3	1:H:200:LEU:HD11	1.96	0.47
1:D:90:GLY:O	1:D:94:VAL:HG23	2.13	0.47
1:E:28:ASN:HA	1:E:57:GLU:OE2	2.15	0.47
1:S:143:MET:HG3	1:S:144:LEU:N	2.30	0.47
1:J:86:MET:HE2	1:J:106:VAL:HG11	1.95	0.47
1:C:120:LYS:NZ	1:D:21:ILE:O	2.47	0.47
1:P:95:LYS:HG3	1:Q:20:GLY:HA3	1.97	0.47
1:B:25:VAL:HG23	1:B:50:VAL:HG11	1.97	0.47
1:J:27:THR:HB	1:J:55:SER:O	2.14	0.47
1:E:130:VAL:HG11	1:E:141:MET:CE	2.43	0.47
1:C:9:ASN:HB3	1:C:12:GLU:HG2	1.97	0.47
1:F:20:GLY:HA3	1:J:95:LYS:HD2	1.97	0.47
1:D:19:TRP:HB3	1:D:21:ILE:HD12	1.97	0.47
1:S:117:LEU:HD22	1:T:21:ILE:HD13	1.97	0.47
1:A:165:ILE:HG12	1:A:182:VAL:HG23	1.97	0.47
1:F:113:ALA:HB1	1:G:192:LEU:HD22	1.97	0.47
1:D:7:THR:CG2	4:D:226:HOH:O	2.54	0.47
1:Q:133:MET:HG3	1:Q:143:MET:HE2	1.96	0.47
1:G:2:LYS:HB2	1:G:181:ILE:HG12	1.96	0.47
1:L:29:PRO:HD3	1:L:57:GLU:HG3	1.96	0.47
1:J:2:LYS:HB2	1:J:181:ILE:HG12	1.97	0.47
1:I:184:MET:HE3	1:I:188:VAL:HG12	1.97	0.47
1:O:31:LEU:HD12	1:O:31:LEU:H	1.80	0.47
1:B:142:ARG:O	1:B:146:GLU:HG3	2.15	0.47
1:B:188:VAL:O	1:B:192:LEU:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:NZ	1:B:2:LYS:HA	2.30	0.46
1:J:184:MET:HE2	1:J:189:LEU:CB	2.45	0.46
1:O:144:LEU:HG	1:O:177:MET:HE1	1.96	0.46
1:Q:213:LEU:N	1:Q:213:LEU:HD12	2.30	0.46
1:G:95:LYS:NZ	1:H:17:VAL:O	2.31	0.46
1:R:72:GLU:O	1:R:75:GLN:OE1	2.33	0.46
1:L:143:MET:HG3	1:L:144:LEU:N	2.30	0.46
1:G:212:TYR:O	1:G:213:LEU:C	2.53	0.46
1:C:203:GLU:O	1:C:207:GLU:HB2	2.16	0.46
1:M:184:MET:HE3	1:M:188:VAL:CG1	2.45	0.46
1:K:19:TRP:HB3	1:K:21:ILE:HD12	1.98	0.46
1:L:142:ARG:NE	1:S:142:ARG:HD2	2.30	0.46
1:N:7:THR:CA	1:N:31:LEU:HD13	2.46	0.46
1:K:131:GLY:O	1:K:135:ASP:OD2	2.34	0.46
1:P:144:LEU:HD21	1:P:179:VAL:HG21	1.98	0.46
1:O:188:VAL:O	1:O:192:LEU:HD13	2.15	0.46
1:C:86:MET:HE1	1:C:114:GLN:O	2.16	0.46
1:H:152:ASN:OD1	3:H:219:GOL:C3	2.64	0.45
1:B:128:PRO:HB3	1:B:143:MET:HE3	1.97	0.45
1:G:78:GLU:O	1:G:103:LYS:NZ	2.48	0.45
1:E:32:ILE:HG23	1:E:37:ALA:HB3	1.96	0.45
1:T:13:ILE:HD12	1:T:50:VAL:CG2	2.46	0.45
1:K:86:MET:CE	1:K:106:VAL:HG11	2.47	0.45
1:R:25:VAL:CG2	1:R:50:VAL:HG21	2.46	0.45
1:M:184:MET:HE2	1:M:189:LEU:N	2.31	0.45
1:S:184:MET:HE2	1:S:189:LEU:N	2.31	0.45
1:N:5:LEU:HB3	1:N:7:THR:HG22	1.98	0.45
1:J:46:ILE:O	1:J:50:VAL:HG23	2.17	0.45
1:Q:188:VAL:O	1:Q:192:LEU:HD13	2.16	0.45
1:I:28:ASN:ND2	1:I:30:THR:OG1	2.35	0.45
1:C:6:ASP:OD1	1:C:183:THR:OG1	2.31	0.45
1:J:6:ASP:OD1	1:J:31:LEU:HD11	2.15	0.45
1:J:55:SER:HB3	1:J:83:LYS:HG3	1.99	0.45
1:Q:130:VAL:HG11	1:Q:141:MET:HE2	1.99	0.45
1:F:140:GLY:O	1:F:143:MET:HG3	2.16	0.45
1:K:110:PHE:CE2	1:K:129:PHE:HB2	2.52	0.45
1:Q:212:TYR:O	1:Q:212:TYR:CG	2.69	0.45
1:N:134:ASP:OD1	1:N:140:GLY:N	2.46	0.45
1:I:210:LYS:HA	1:I:213:LEU:HD12	1.99	0.45
1:M:166:ARG:H	1:M:170:HIS:CD2	2.33	0.45
1:T:165:ILE:HD12	1:T:170:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:8:ALA:HB3	1:I:31:LEU:O	2.17	0.45
1:C:144:LEU:HD23	1:C:177:MET:HE1	1.98	0.45
1:M:4:PHE:CZ	1:M:53:PRO:HG2	2.52	0.45
1:B:184:MET:HE1	1:B:192:LEU:HD22	1.99	0.44
1:O:144:LEU:HD21	1:O:179:VAL:HG21	1.99	0.44
1:I:63:TYR:O	1:I:67:VAL:HG23	2.17	0.44
1:J:31:LEU:O	1:J:35:GLU:CG	2.58	0.44
1:J:2:LYS:HA	1:J:23:ASP:OD2	2.17	0.44
1:S:12:GLU:HB2	1:S:186:PHE:CD1	2.52	0.44
1:R:174:ALA:HB1	1:R:179:VAL:CG2	2.48	0.44
1:Q:2:LYS:HB2	1:Q:181:ILE:HG23	1.99	0.44
1:F:10:LEU:HD22	1:F:49:LEU:HD12	1.99	0.44
1:H:39:PHE:HB2	1:I:212:TYR:OH	2.17	0.44
1:I:147:ILE:HG22	1:I:160:ILE:HD13	2.00	0.44
1:O:148:VAL:HG21	1:O:179:VAL:HG22	2.00	0.44
1:M:86:MET:HE1	1:M:118:ALA:HB2	1.99	0.44
1:F:21:ILE:CD1	1:J:91:ILE:HG21	2.47	0.44
1:O:180:ASP:OD1	3:O:220:GOL:O1	2.33	0.44
1:A:120:LYS:NZ	1:B:1:MET:O	2.47	0.44
1:Q:82:ILE:HD13	1:Q:102:ILE:CG2	2.47	0.44
1:B:167:HIS:CD2	4:B:220:HOH:O	2.70	0.44
1:O:7:THR:HG23	1:O:13:ILE:HD11	2.00	0.44
1:Q:19:TRP:HB2	1:Q:21:ILE:HG12	1.98	0.44
1:P:3:ILE:HD12	1:T:120:LYS:HD3	2.00	0.44
1:J:125:TYR:CD2	1:J:161:ILE:HD11	2.52	0.44
1:C:174:ALA:HB1	1:C:179:VAL:HG11	2.00	0.44
1:D:2:LYS:HB2	1:D:181:ILE:HG12	2.00	0.44
1:B:143:MET:HE3	1:B:147:ILE:CD1	2.48	0.43
1:I:10:LEU:HD23	1:I:13:ILE:HD12	2.00	0.43
1:L:88:PRO:HA	1:M:193:PHE:CE2	2.53	0.43
1:H:149:GLU:HG2	1:I:176:LEU:CD2	2.48	0.43
1:C:27:THR:O	1:C:83:LYS:HE2	2.17	0.43
1:B:82:ILE:HD12	1:B:102:ILE:CG2	2.48	0.43
1:H:57:GLU:HA	1:H:83:LYS:HB2	2.01	0.43
1:I:63:TYR:CE1	1:I:67:VAL:HG21	2.54	0.43
1:N:87:THR:HB	1:N:88:PRO:HD2	2.00	0.43
1:N:113:ALA:HB1	1:O:192:LEU:HG	1.99	0.43
1:D:2:LYS:HB2	1:D:181:ILE:HG23	1.99	0.43
1:J:100:GLU:HG3	1:J:102:ILE:HD12	1.99	0.43
1:I:184:MET:HE1	1:I:189:LEU:HA	1.99	0.43
1:Q:202:ILE:O	1:Q:206:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:120:LYS:NZ	1:Q:2:LYS:HA	2.34	0.43
1:Q:-1:HIS:CG	1:Q:0:HIS:N	2.86	0.43
1:S:4:PHE:CZ	1:S:181:ILE:HD13	2.53	0.43
1:S:86:MET:HE3	1:S:114:GLN:O	2.18	0.43
1:J:46:ILE:HG22	1:J:54:VAL:HG21	2.01	0.43
1:S:13:ILE:O	1:S:17:VAL:HG13	2.18	0.43
1:E:57:GLU:CD	1:E:83:LYS:NZ	2.72	0.43
1:O:137:SER:HB2	1:P:111:SER:HB2	1.99	0.43
1:C:188:VAL:O	1:C:192:LEU:HD13	2.19	0.43
1:J:28:ASN:HB2	1:J:31:LEU:HD12	2.00	0.43
1:E:205:PHE:CD1	1:E:206:MET:N	2.87	0.43
1:M:110:PHE:CE1	1:M:129:PHE:HB2	2.53	0.43
1:E:184:MET:HE2	1:E:189:LEU:CB	2.49	0.42
1:O:28:ASN:HB3	1:O:31:LEU:CD1	2.49	0.42
1:E:28:ASN:HB2	1:E:29:PRO:HD2	2.00	0.42
1:E:86:MET:HE1	1:E:118:ALA:HB2	2.01	0.42
1:I:128:PRO:HB3	1:I:143:MET:HE1	2.01	0.42
1:K:57:GLU:HA	1:K:83:LYS:HB2	2.00	0.42
1:I:90:GLY:O	1:I:94:VAL:HG23	2.18	0.42
1:B:143:MET:CE	1:B:147:ILE:HD11	2.49	0.42
1:Q:55:SER:HA	1:Q:81:VAL:O	2.19	0.42
1:I:94:VAL:O	1:I:98:SER:OG	2.31	0.42
1:K:184:MET:HE1	1:K:189:LEU:CA	2.49	0.42
1:Q:113:ALA:HB1	1:R:192:LEU:HG	2.01	0.42
1:O:148:VAL:CG2	1:O:179:VAL:HG22	2.49	0.42
1:R:154:TYR:OH	1:S:179:VAL:O	2.31	0.42
1:T:104:THR:O	1:T:124:THR:HB	2.19	0.42
1:D:7:THR:CG2	1:D:12:GLU:OE1	2.64	0.42
1:B:141:MET:HE3	1:B:177:MET:SD	2.59	0.42
1:D:87:THR:HB	1:D:88:PRO:HD2	2.00	0.42
1:N:9:ASN:HB3	1:N:12:GLU:HG2	2.01	0.42
1:E:172:VAL:HG21	1:G:137:SER:HB3	2.02	0.42
1:K:28:ASN:C	1:K:28:ASN:ND2	2.71	0.42
1:E:86:MET:HE2	1:E:106:VAL:CG1	2.49	0.42
1:K:20:GLY:HA3	1:O:95:LYS:HG3	2.01	0.42
1:N:149:GLU:HA	1:N:149:GLU:OE1	2.19	0.42
1:E:5:LEU:HB3	1:E:7:THR:HG22	2.00	0.42
1:L:9:ASN:HB3	1:L:12:GLU:HG2	2.02	0.42
1:D:52:GLY:O	1:D:79:TYR:HB3	2.19	0.42
1:N:184:MET:CE	1:N:192:LEU:HD11	2.50	0.42
1:R:13:ILE:CG2	1:R:50:VAL:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:90:GLY:O	1:O:94:VAL:HG23	2.19	0.42
1:F:3:ILE:HD12	1:J:120:LYS:HE2	2.02	0.42
1:I:110:PHE:CE1	1:I:129:PHE:HB2	2.55	0.42
1:Q:91:ILE:HG21	1:R:21:ILE:HD11	2.02	0.42
1:O:171:VAL:HG21	1:O:184:MET:HE3	2.01	0.42
1:C:144:LEU:CD2	1:C:177:MET:HE1	2.50	0.42
1:M:51:LYS:HA	1:M:79:TYR:CE2	2.55	0.42
1:M:5:LEU:HB3	1:M:7:THR:HG22	2.02	0.42
1:C:39:PHE:O	1:C:43:VAL:HG23	2.20	0.42
1:R:69:GLU:O	1:R:73:LEU:HG	2.19	0.41
1:I:27:THR:O	1:I:83:LYS:NZ	2.43	0.41
1:O:91:ILE:HG23	1:O:121:ALA:HB2	2.02	0.41
1:R:9:ASN:HB3	1:R:12:GLU:HG3	2.02	0.41
1:M:195:HIS:CG	1:M:196:PRO:HD2	2.55	0.41
1:I:32:ILE:CG2	1:I:32:ILE:O	2.69	0.41
1:A:28:ASN:CB	1:A:29:PRO:CD	2.97	0.41
1:G:95:LYS:HZ1	1:H:20:GLY:HA2	1.85	0.41
1:S:30:THR:HG23	1:T:208:ASP:HB3	2.00	0.41
1:K:82:ILE:HD13	1:K:102:ILE:CG2	2.50	0.41
1:H:28:ASN:HB2	1:H:29:PRO:CD	2.50	0.41
1:L:116:ILE:HD11	1:L:150:ILE:HD13	2.02	0.41
1:P:29:PRO:O	1:P:33:SER:HB2	2.20	0.41
1:D:80:VAL:HG13	1:D:80:VAL:O	2.19	0.41
1:S:91:ILE:HG21	1:T:21:ILE:HD11	2.03	0.41
1:S:55:SER:HB3	1:S:83:LYS:HG3	2.02	0.41
1:P:88:PRO:HA	1:Q:193:PHE:CE2	2.55	0.41
1:A:26:THR:CG2	1:A:83:LYS:NZ	2.83	0.41
1:R:9:ASN:HB3	1:R:12:GLU:CG	2.51	0.41
1:N:83:LYS:HG2	1:N:107:THR:HG21	2.02	0.41
1:P:1:MET:HE3	1:P:175:ALA:CA	2.48	0.41
1:R:86:MET:O	1:S:198:THR:HG21	2.20	0.41
1:K:165:ILE:HD12	1:K:170:HIS:HB3	2.02	0.41
1:O:110:PHE:CE1	1:O:129:PHE:HB2	2.55	0.41
1:H:184:MET:HE2	1:H:189:LEU:CB	2.50	0.41
1:L:-1:HIS:ND1	1:L:2:LYS:HE2	2.35	0.41
1:L:0:HIS:HB2	1:L:2:LYS:HZ3	1.84	0.41
1:P:140:GLY:O	1:P:143:MET:HG3	2.21	0.41
1:B:113:ALA:HB1	1:C:192:LEU:HG	2.03	0.41
1:P:104:THR:O	1:P:124:THR:HB	2.21	0.41
1:H:19:TRP:HB3	1:H:21:ILE:HD13	2.03	0.41
1:O:21:ILE:HD13	1:O:21:ILE:HG21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:SER:HA	1:C:81:VAL:O	2.21	0.41
1:E:130:VAL:HG11	1:E:141:MET:HE2	2.03	0.41
1:P:143:MET:HG3	1:P:144:LEU:N	2.35	0.41
1:E:205:PHE:CD1	1:E:205:PHE:C	2.94	0.41
1:O:27:THR:O	1:O:83:LYS:HE3	2.21	0.41
1:B:149:GLU:HG2	1:C:176:LEU:HD23	2.03	0.41
1:J:86:MET:HE2	1:J:106:VAL:CG1	2.51	0.40
1:D:21:ILE:HG21	1:D:21:ILE:HD13	1.88	0.40
1:T:167:HIS:HB2	1:T:168:PRO:CD	2.51	0.40
1:G:25:VAL:O	1:G:54:VAL:HA	2.20	0.40
1:A:151:TYR:HB3	3:A:219:GOL:H32	2.03	0.40
1:B:52:GLY:O	1:B:54:VAL:HG23	2.21	0.40
1:J:29:PRO:O	1:J:33:SER:N	2.51	0.40
1:I:143:MET:HE1	1:I:147:ILE:HD12	2.03	0.40
1:B:90:GLY:O	1:B:94:VAL:HG23	2.22	0.40
1:L:63:TYR:HE1	1:L:93:ALA:HA	1.86	0.40
1:T:212:TYR:C	1:T:212:TYR:CD1	2.94	0.40
1:K:86:MET:HE2	1:K:91:ILE:HD11	2.03	0.40
1:T:174:ALA:HB1	1:T:179:VAL:HG11	2.03	0.40
1:C:2:LYS:HB2	1:C:181:ILE:HG12	2.04	0.40
1:D:96:THR:O	1:D:100:GLU:HG3	2.21	0.40
1:S:174:ALA:O	1:S:179:VAL:HG23	2.21	0.40
1:P:32:ILE:HD13	1:P:39:PHE:HD1	1.86	0.40
1:E:167:HIS:O	1:E:170:HIS:HB2	2.21	0.40
1:T:143:MET:HG3	1:T:144:LEU:N	2.37	0.40
1:K:86:MET:CE	1:K:91:ILE:HD11	2.50	0.40
1:M:167:HIS:NE2	1:M:170:HIS:CE1	2.89	0.40
1:C:86:MET:CE	1:C:114:GLN:O	2.69	0.40
1:O:148:VAL:HG21	1:O:177:MET:CE	2.51	0.40

There are no symmetry-related clashes.

## 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	203/230 (88%)	198 (98%)	5 (2%)	0	100	100
1	B	207/230 (90%)	205 (99%)	2 (1%)	0	100	100
1	C	206/230 (90%)	202 (98%)	3 (2%)	1 (0%)	34	48
1	D	208/230 (90%)	204 (98%)	3 (1%)	1 (0%)	34	48
1	E	214/230 (93%)	210 (98%)	2 (1%)	2 (1%)	21	30
1	F	209/230 (91%)	204 (98%)	5 (2%)	0	100	100
1	G	214/230 (93%)	210 (98%)	3 (1%)	1 (0%)	34	48
1	H	201/230 (87%)	196 (98%)	4 (2%)	1 (0%)	34	48
1	I	207/230 (90%)	202 (98%)	4 (2%)	1 (0%)	34	48
1	J	211/230 (92%)	207 (98%)	4 (2%)	0	100	100
1	K	214/230 (93%)	212 (99%)	2 (1%)	0	100	100
1	L	200/230 (87%)	194 (97%)	5 (2%)	1 (0%)	34	48
1	M	194/230 (84%)	191 (98%)	3 (2%)	0	100	100
1	N	200/230 (87%)	195 (98%)	5 (2%)	0	100	100
1	O	208/230 (90%)	204 (98%)	4 (2%)	0	100	100
1	P	207/230 (90%)	201 (97%)	5 (2%)	1 (0%)	34	48
1	Q	205/230 (89%)	201 (98%)	3 (2%)	1 (0%)	34	48
1	R	206/230 (90%)	200 (97%)	5 (2%)	1 (0%)	34	48
1	S	203/230 (88%)	199 (98%)	2 (1%)	2 (1%)	19	28
1	T	200/230 (87%)	197 (98%)	2 (1%)	1 (0%)	34	48
All	All	4117/4600 (90%)	4032 (98%)	71 (2%)	14 (0%)	46	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	0	HIS
1	P	41	GLN
1	S	38	GLU
1	E	41	GLN
1	H	204	ARG
1	R	213	LEU
1	S	39	PHE
1	C	39	PHE
1	E	39	PHE
1	L	31	LEU
1	D	0	HIS

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Mol	Chain	Res	Type
1	I	213	LEU
1	Q	212	TYR
1	T	29	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	171/196 (87%)	158 (92%)	13 (8%)	16	25
1	B	168/196 (86%)	154 (92%)	14 (8%)	14	21
1	C	165/196 (84%)	152 (92%)	13 (8%)	15	23
1	D	175/196 (89%)	166 (95%)	9 (5%)	29	46
1	E	181/196 (92%)	171 (94%)	10 (6%)	27	42
1	F	179/196 (91%)	163 (91%)	16 (9%)	12	18
1	G	179/196 (91%)	170 (95%)	9 (5%)	30	48
1	H	166/196 (85%)	152 (92%)	14 (8%)	14	20
1	I	173/196 (88%)	164 (95%)	9 (5%)	29	45
1	J	172/196 (88%)	157 (91%)	15 (9%)	13	19
1	K	176/196 (90%)	165 (94%)	11 (6%)	22	35
1	L	161/196 (82%)	144 (89%)	17 (11%)	8	12
1	M	152/196 (78%)	141 (93%)	11 (7%)	18	28
1	N	151/196 (77%)	140 (93%)	11 (7%)	17	27
1	O	173/196 (88%)	162 (94%)	11 (6%)	22	34
1	P	167/196 (85%)	155 (93%)	12 (7%)	18	28
1	Q	168/196 (86%)	161 (96%)	7 (4%)	36	56
1	R	167/196 (85%)	152 (91%)	15 (9%)	12	17
1	S	162/196 (83%)	146 (90%)	16 (10%)	10	14
1	T	162/196 (83%)	151 (93%)	11 (7%)	20	31
All	All	3368/3920 (86%)	3124 (93%)	244 (7%)	18	28



All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
1	A	1	MET
1	A	68	ARG
1	A	76	ILE
1	A	95	LYS
1	A	126	VAL
1	A	165	ILE
1	A	166	ARG
1	A	179	VAL
1	A	182	VAL
1	A	192	LEU
1	A	205	PHE
1	A	216	LEU
1	B	15	LYS
1	B	50	VAL
1	B	60	SER
1	B	75	GLN
1	B	92	LYS
1	B	107	THR
1	B	116	ILE
1	B	143	MET
1	B	144	LEU
1	B	149	GLU
1	B	166	ARG
1	B	184	MET
1	B	204	ARG
1	B	206	MET
1	C	27	THR
1	C	30	THR
1	C	50	VAL
1	C	60	SER
1	C	64	GLU
1	C	78	GLU
1	C	126	VAL
1	C	132	ARG
1	C	143	MET
1	C	166	ARG
1	C	182	VAL
1	C	192	LEU
1	C	205	PHE
1	D	27	THR
1	D	30	THR

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Mol	Chain	Res	Type
1	D	58	VAL
1	D	72	GLU
1	D	83	LYS
1	D	136	LEU
1	D	143	MET
1	D	204	ARG
1	D	206	MET
1	E	6	ASP
1	E	15	LYS
1	E	27	THR
1	E	30	THR
1	E	33	SER
1	E	40	LYS
1	E	72	GLU
1	E	142	ARG
1	E	166	ARG
1	E	205	PHE
1	F	0	HIS
1	F	2	LYS
1	F	11	GLU
1	F	21	ILE
1	F	27	THR
1	F	49	LEU
1	F	50	VAL
1	F	58	VAL
1	F	76	ILE
1	F	103	LYS
1	F	116	ILE
1	F	143	MET
1	F	166	ARG
1	F	182	VAL
1	F	204	ARG
1	F	215	ASN
1	G	26	THR
1	G	30	THR
1	G	54	VAL
1	G	143	MET
1	G	166	ARG
1	G	207	GLU
1	G	209	TRP
1	G	210	LYS
1	G	214	GLU

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Mol	Chain	Res	Type
1	H	21	ILE
1	H	27	THR
1	H	30	THR
1	H	33	SER
1	H	42	ARG
1	H	50	VAL
1	H	58	VAL
1	H	60	SER
1	H	72	GLU
1	H	89	ASP
1	H	95	LYS
1	H	111	SER
1	H	143	MET
1	H	166	ARG
1	I	28	ASN
1	I	57	GLU
1	I	58	VAL
1	I	78	GLU
1	I	95	LYS
1	I	98	SER
1	I	120	LYS
1	I	143	MET
1	I	166	ARG
1	J	6	ASP
1	J	10	LEU
1	J	27	THR
1	J	42	ARG
1	J	45	GLU
1	J	49	LEU
1	J	50	VAL
1	J	68	ARG
1	J	75	GLN
1	J	78	GLU
1	J	95	LYS
1	J	126	VAL
1	J	143	MET
1	J	166	ARG
1	J	199	ASP
1	K	12	GLU
1	K	17	VAL
1	K	28	ASN
1	K	30	THR

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Mol	Chain	Res	Type
1	K	58	VAL
1	K	143	MET
1	K	166	ARG
1	K	179	VAL
1	K	184	MET
1	K	204	ARG
1	K	209	TRP
1	L	21	ILE
1	L	27	THR
1	L	28	ASN
1	L	30	THR
1	L	49	LEU
1	L	57	GLU
1	L	58	VAL
1	L	68	ARG
1	L	78	GLU
1	L	107	THR
1	L	124	THR
1	L	126	VAL
1	L	134	ASP
1	L	141	MET
1	L	143	MET
1	L	182	VAL
1	L	208	ASP
1	M	27	THR
1	M	30	THR
1	M	33	SER
1	M	49	LEU
1	M	55	SER
1	M	62	ASP
1	M	68	ARG
1	M	81	VAL
1	M	107	THR
1	M	143	MET
1	M	166	ARG
1	N	0	HIS
1	N	21	ILE
1	N	50	VAL
1	N	55	SER
1	N	58	VAL
1	N	77	SER
1	N	83	LYS

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Mol	Chain	Res	Type
1	N	126	VAL
1	N	141	MET
1	N	166	ARG
1	N	191	LYS
1	O	-1	HIS
1	O	6	ASP
1	O	21	ILE
1	O	27	THR
1	O	30	THR
1	O	35	GLU
1	O	50	VAL
1	O	68	ARG
1	O	95	LYS
1	O	143	MET
1	O	208	ASP
1	P	2	LYS
1	P	15	LYS
1	P	27	THR
1	P	33	SER
1	P	40	LYS
1	P	42	ARG
1	P	49	LEU
1	P	95	LYS
1	P	126	VAL
1	P	142	ARG
1	P	143	MET
1	P	166	ARG
1	Q	27	THR
1	Q	28	ASN
1	Q	64	GLU
1	Q	72	GLU
1	Q	192	LEU
1	Q	204	ARG
1	Q	209	TRP
1	R	0	HIS
1	R	12	GLU
1	R	27	THR
1	R	59	VAL
1	R	75	GLN
1	R	87	THR
1	R	107	THR
1	R	116	ILE

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Mol	Chain	Res	Type
1	R	142	ARG
1	R	143	MET
1	R	166	ARG
1	R	179	VAL
1	R	182	VAL
1	R	192	LEU
1	R	209	TRP
1	S	2	LYS
1	S	5	LEU
1	S	27	THR
1	S	30	THR
1	S	50	VAL
1	S	68	ARG
1	S	89	ASP
1	S	95	LYS
1	S	120	LYS
1	S	126	VAL
1	S	142	ARG
1	S	143	MET
1	S	166	ARG
1	S	177	MET
1	S	184	MET
1	S	204	ARG
1	T	2	LYS
1	T	27	THR
1	T	60	SER
1	T	62	ASP
1	T	75	GLN
1	T	95	LYS
1	T	103	LYS
1	T	104	THR
1	T	143	MET
1	T	161	ILE
1	T	204	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	167	HIS
1	K	28	ASN
1	L	28	ASN
1	M	170	HIS

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Mol	Chain	Res	Type
1	N	0	HIS
1	N	167	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 ⓘ

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	A	219	-	5,5,5	0.53	0	5,5,5	1.09	0
3	GOL	B	219	-	5,5,5	0.39	0	5,5,5	0.82	0
3	GOL	C	219	-	5,5,5	0.42	0	5,5,5	1.17	0
3	GOL	D	219	-	5,5,5	0.27	0	5,5,5	1.02	0
3	GOL	E	219	-	5,5,5	0.24	0	5,5,5	0.80	0
3	GOL	F	219	-	5,5,5	0.36	0	5,5,5	0.28	0
3	GOL	G	219	-	5,5,5	0.77	0	5,5,5	1.26	1 (20%)
3	GOL	H	219	-	5,5,5	0.39	0	5,5,5	1.03	0
3	GOL	I	219	-	5,5,5	0.17	0	5,5,5	0.57	0
3	GOL	J	219	-	5,5,5	0.13	0	5,5,5	0.71	0
3	GOL	K	219[A]	-	5,5,5	0.21	0	5,5,5	0.57	0
3	GOL	K	219[B]	-	5,5,5	0.38	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	L	219	-	5,5,5	0.27	0	5,5,5	0.26	0
3	GOL	M	219	-	5,5,5	0.37	0	5,5,5	0.83	0
3	GOL	N	219	-	5,5,5	0.16	0	5,5,5	0.64	0
2	SO4	O	219	-	4,4,4	0.20	0	6,6,6	0.19	0
3	GOL	O	220	-	5,5,5	0.50	0	5,5,5	1.43	1 (20%)
3	GOL	P	219	-	5,5,5	0.30	0	5,5,5	0.39	0
3	GOL	P	220	-	5,5,5	0.24	0	5,5,5	0.76	0
3	GOL	Q	219	-	5,5,5	0.39	0	5,5,5	0.83	0
3	GOL	R	219	-	5,5,5	0.28	0	5,5,5	0.76	0
3	GOL	S	219	-	5,5,5	0.37	0	5,5,5	0.63	0
3	GOL	T	219	-	5,5,5	0.41	0	5,5,5	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	219	-	-	0/4/4/4	0/0/0/0
3	GOL	B	219	-	-	0/4/4/4	0/0/0/0
3	GOL	C	219	-	-	0/4/4/4	0/0/0/0
3	GOL	D	219	-	-	0/4/4/4	0/0/0/0
3	GOL	E	219	-	-	0/4/4/4	0/0/0/0
3	GOL	F	219	-	-	0/4/4/4	0/0/0/0
3	GOL	G	219	-	-	0/4/4/4	0/0/0/0
3	GOL	H	219	-	-	0/4/4/4	0/0/0/0
3	GOL	I	219	-	-	0/4/4/4	0/0/0/0
3	GOL	J	219	-	-	0/4/4/4	0/0/0/0
3	GOL	K	219[A]	-	-	0/4/4/4	0/0/0/0
3	GOL	K	219[B]	-	-	0/4/4/4	0/0/0/0
3	GOL	L	219	-	-	0/4/4/4	0/0/0/0
3	GOL	M	219	-	-	0/4/4/4	0/0/0/0
3	GOL	N	219	-	-	0/4/4/4	0/0/0/0
2	SO4	O	219	-	-	0/0/0/0	0/0/0/0
3	GOL	O	220	-	-	0/4/4/4	0/0/0/0
3	GOL	P	219	-	-	0/4/4/4	0/0/0/0
3	GOL	P	220	-	-	0/4/4/4	0/0/0/0
3	GOL	Q	219	-	-	0/4/4/4	0/0/0/0
3	GOL	R	219	-	-	0/4/4/4	0/0/0/0
3	GOL	S	219	-	-	0/4/4/4	0/0/0/0
3	GOL	T	219	-	-	0/4/4/4	0/0/0/0



There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	220	GOL	C3-C2-C1	-2.29	102.14	111.12
3	G	219	GOL	O1-C1-C2	2.35	121.56	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	219	GOL	1	0
3	B	219	GOL	1	0
3	C	219	GOL	1	0
3	F	219	GOL	1	0
3	H	219	GOL	2	0
3	O	220	GOL	3	0
3	P	220	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	207/230 (90%)	0.27	3 (1%) 78 77	36, 49, 59, 81	0
1	B	209/230 (90%)	0.12	2 (0%) 84 83	39, 49, 67, 79	0
1	C	208/230 (90%)	0.11	3 (1%) 78 77	40, 49, 60, 73	0
1	D	210/230 (91%)	0.15	2 (0%) 84 83	40, 49, 65, 86	0
1	E	216/230 (93%)	0.12	1 (0%) 91 91	41, 49, 60, 75	0
1	F	213/230 (92%)	0.10	2 (0%) 85 85	39, 49, 61, 87	0
1	G	216/230 (93%)	0.16	2 (0%) 85 85	40, 49, 61, 89	0
1	H	205/230 (89%)	0.08	2 (0%) 84 83	38, 49, 60, 70	0
1	I	211/230 (91%)	0.18	5 (2%) 62 61	41, 48, 60, 83	0
1	J	213/230 (92%)	0.25	4 (1%) 70 69	37, 49, 72, 83	0
1	K	216/230 (93%)	0.24	4 (1%) 70 69	39, 48, 61, 69	0
1	L	204/230 (88%)	0.34	11 (5%) 29 30	37, 48, 57, 85	0
1	M	198/230 (86%)	0.22	6 (3%) 54 53	40, 48, 60, 68	0
1	N	204/230 (88%)	0.28	10 (4%) 33 34	40, 48, 57, 66	0
1	O	210/230 (91%)	0.25	7 (3%) 50 50	39, 48, 65, 82	0
1	P	209/230 (90%)	0.07	0 100 100	39, 49, 60, 84	0
1	Q	208/230 (90%)	0.13	5 (2%) 62 61	39, 48, 60, 74	0
1	R	210/230 (91%)	0.45	18 (8%) 13 13	40, 49, 61, 74	0
1	S	205/230 (89%)	0.27	4 (1%) 68 68	40, 48, 60, 72	0
1	T	204/230 (88%)	0.41	13 (6%) 23 23	40, 48, 57, 66	0
All	All	4176/4600 (90%)	0.21	104 (2%) 61 60	36, 49, 61, 89	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	209	TRP	8.9
1	H	32	ILE	6.1
1	M	91	ILE	5.5
1	T	205	PHE	5.5
1	R	209	TRP	4.8
1	O	10	LEU	4.7
1	S	32	ILE	4.5
1	O	36	GLY	4.4
1	O	11	GLU	4.1
1	J	36	GLY	4.0
1	O	37	ALA	4.0
1	R	79	TYR	4.0
1	N	8	ALA	3.9
1	N	32	ILE	3.9
1	L	59	VAL	3.6
1	I	68	ARG	3.6
1	G	32	ILE	3.6
1	R	82	ILE	3.5
1	R	205	PHE	3.5
1	L	75	GLN	3.4
1	R	102	ILE	3.4
1	D	32	ILE	3.4
1	N	47	CYS	3.4
1	T	79	TYR	3.3
1	T	50	VAL	3.3
1	R	59	VAL	3.3
1	R	208	ASP	3.2
1	R	70	ALA	3.2
1	C	32	ILE	3.2
1	Q	59	VAL	3.2
1	T	8	ALA	3.2
1	J	206	MET	3.2
1	R	213	LEU	3.1
1	R	212	TYR	3.0
1	N	49	LEU	3.0
1	F	209	TRP	3.0
1	O	32	ILE	2.9
1	T	52	GLY	2.8
1	M	8	ALA	2.8
1	T	19	TRP	2.8
1	R	75	GLN	2.8
1	R	206	MET	2.8
1	K	67	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	T	27	THR	2.8
1	F	61	LEU	2.7
1	R	207	GLU	2.7
1	T	212	TYR	2.7
1	S	36	GLY	2.7
1	I	78	GLU	2.6
1	Q	205	PHE	2.6
1	I	58	VAL	2.6
1	T	209	TRP	2.6
1	N	52	GLY	2.5
1	T	21	ILE	2.5
1	L	66	MET	2.5
1	G	37	ALA	2.5
1	M	80	VAL	2.5
1	N	91	ILE	2.5
1	R	124	THR	2.5
1	J	205	PHE	2.5
1	I	8	ALA	2.5
1	B	33	SER	2.5
1	K	46	ILE	2.4
1	T	75	GLN	2.4
1	T	49	LEU	2.4
1	R	60	SER	2.4
1	L	60	SER	2.4
1	O	49	LEU	2.3
1	L	79	TYR	2.3
1	N	187	ALA	2.3
1	D	205	PHE	2.3
1	L	11	GLU	2.3
1	C	205	PHE	2.3
1	A	6	ASP	2.3
1	R	68	ARG	2.2
1	N	21	ILE	2.2
1	L	12	GLU	2.2
1	C	36	GLY	2.2
1	K	209	TRP	2.2
1	H	39	PHE	2.2
1	L	54	VAL	2.2
1	S	39	PHE	2.2
1	N	46	ILE	2.2
1	E	36	GLY	2.1
1	B	32	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	32	ILE	2.1
1	J	209	TRP	2.1
1	Q	99	ALA	2.1
1	A	48	ASP	2.1
1	M	48	ASP	2.1
1	R	78	GLU	2.1
1	O	205	PHE	2.1
1	R	73	LEU	2.1
1	M	30	THR	2.1
1	L	25	VAL	2.1
1	L	96	THR	2.1
1	T	96	THR	2.1
1	I	208	ASP	2.1
1	Q	37	ALA	2.0
1	A	41	GLN	2.0
1	L	58	VAL	2.0
1	M	49	LEU	2.0
1	N	54	VAL	2.0
1	S	82	ILE	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	SO4	O	219	5/5	0.80	0.27	10.33	91,92,96,103	0
3	GOL	H	219	6/6	0.81	0.23	2.04	49,55,58,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	R	219	6/6	0.83	0.21	1.70	61,70,76,81	0
3	GOL	C	219	6/6	0.85	0.19	1.58	58,60,68,71	0
3	GOL	N	219	6/6	0.79	0.17	1.44	61,67,68,74	0
3	GOL	E	219	6/6	0.85	0.19	1.15	33,49,51,65	0
3	GOL	D	219	6/6	0.88	0.19	0.98	52,58,64,65	0
3	GOL	F	219	6/6	0.84	0.19	0.80	60,62,62,69	0
3	GOL	K	219[A]	6/6	0.89	0.18	0.74	38,46,48,53	4
3	GOL	P	219	6/6	0.87	0.18	0.50	54,73,81,85	0
3	GOL	O	220	6/6	0.86	0.17	0.45	47,49,53,62	0
3	GOL	G	219	6/6	0.78	0.19	0.44	34,49,53,57	0
3	GOL	K	219[B]	6/6	0.89	0.18	0.30	34,45,48,53	4
3	GOL	Q	219	6/6	0.86	0.17	0.11	44,52,62,64	0
3	GOL	L	219	6/6	0.85	0.17	0.07	85,90,93,94	0
3	GOL	M	219	6/6	0.84	0.15	-0.09	74,77,77,81	0
3	GOL	T	219	6/6	0.92	0.15	-0.19	54,67,71,74	0
3	GOL	B	219	6/6	0.92	0.15	-0.32	41,55,67,68	0
3	GOL	S	219	6/6	0.86	0.13	-0.83	61,65,67,70	0
3	GOL	J	219	6/6	0.92	0.13	-1.20	42,53,62,68	0
3	GOL	P	220	6/6	0.89	0.14	-1.65	45,54,59,59	0
3	GOL	A	219	6/6	0.94	0.12	-1.66	42,57,58,58	0
3	GOL	I	219	6/6	0.94	0.08	-3.10	51,56,59,62	0

## 6.5 Other polymers

There are no such residues in this entry.