



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:43 pm BST

PDB ID : 4JEK  
Title : Structure of dibenzothiophene monooxygenase (DszC) from *Rhodococcus erythropolis*  
Authors : Zhang, L.; Duan, X.L.; Zhou, D.M.; Li, X.  
Deposited on : 2013-02-27  
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

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

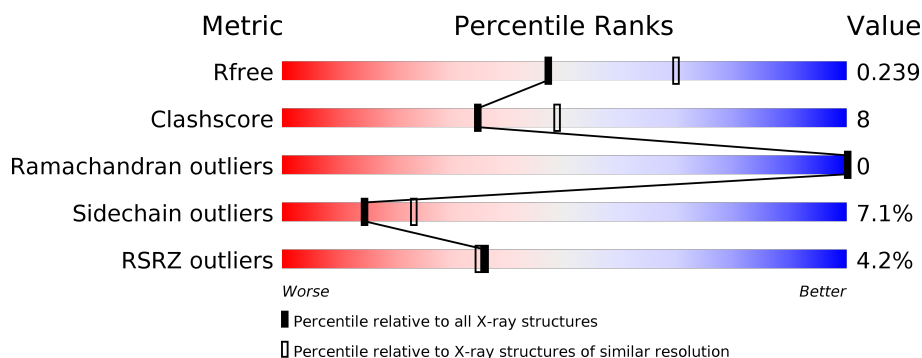
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	
1	C	453	
1	D	453	
1	E	453	
1	F	453	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	453	<div><div>%</div><div><div></div><div>70%</div><div>16%</div><div>•</div><div>12%</div></div></div>
1	H	453	<div><div>4%</div><div><div></div><div>68%</div><div>18%</div><div>•</div><div>12%</div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24898 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 Dibenzothiophene desulfurization enzyme C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	B	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	C	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	D	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	E	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	F	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	G	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			
1	H	399	Total	C	N	O	S	0	0	0
			3041	1911	540	586	4			

There are 288 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	EXPRESSION TAG	UNP P54998
A	-34	GLY	-	EXPRESSION TAG	UNP P54998
A	-33	SER	-	EXPRESSION TAG	UNP P54998
A	-32	SER	-	EXPRESSION TAG	UNP P54998
A	-31	HIS	-	EXPRESSION TAG	UNP P54998
A	-30	HIS	-	EXPRESSION TAG	UNP P54998
A	-29	HIS	-	EXPRESSION TAG	UNP P54998
A	-28	HIS	-	EXPRESSION TAG	UNP P54998
A	-27	HIS	-	EXPRESSION TAG	UNP P54998
A	-26	HIS	-	EXPRESSION TAG	UNP P54998
A	-25	SER	-	EXPRESSION TAG	UNP P54998
A	-24	SER	-	EXPRESSION TAG	UNP P54998
A	-23	GLY	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	LEU	-	EXPRESSION TAG	UNP P54998
A	-21	VAL	-	EXPRESSION TAG	UNP P54998
A	-20	PRO	-	EXPRESSION TAG	UNP P54998
A	-19	ARG	-	EXPRESSION TAG	UNP P54998
A	-18	GLY	-	EXPRESSION TAG	UNP P54998
A	-17	SER	-	EXPRESSION TAG	UNP P54998
A	-16	HIS	-	EXPRESSION TAG	UNP P54998
A	-15	MET	-	EXPRESSION TAG	UNP P54998
A	-14	ALA	-	EXPRESSION TAG	UNP P54998
A	-13	SER	-	EXPRESSION TAG	UNP P54998
A	-12	MET	-	EXPRESSION TAG	UNP P54998
A	-11	THR	-	EXPRESSION TAG	UNP P54998
A	-10	GLY	-	EXPRESSION TAG	UNP P54998
A	-9	GLY	-	EXPRESSION TAG	UNP P54998
A	-8	GLN	-	EXPRESSION TAG	UNP P54998
A	-7	GLN	-	EXPRESSION TAG	UNP P54998
A	-6	MET	-	EXPRESSION TAG	UNP P54998
A	-5	GLY	-	EXPRESSION TAG	UNP P54998
A	-4	ARG	-	EXPRESSION TAG	UNP P54998
A	-3	GLY	-	EXPRESSION TAG	UNP P54998
A	-2	SER	-	EXPRESSION TAG	UNP P54998
A	-1	GLU	-	EXPRESSION TAG	UNP P54998
A	0	PHE	-	EXPRESSION TAG	UNP P54998
B	-35	MET	-	EXPRESSION TAG	UNP P54998
B	-34	GLY	-	EXPRESSION TAG	UNP P54998
B	-33	SER	-	EXPRESSION TAG	UNP P54998
B	-32	SER	-	EXPRESSION TAG	UNP P54998
B	-31	HIS	-	EXPRESSION TAG	UNP P54998
B	-30	HIS	-	EXPRESSION TAG	UNP P54998
B	-29	HIS	-	EXPRESSION TAG	UNP P54998
B	-28	HIS	-	EXPRESSION TAG	UNP P54998
B	-27	HIS	-	EXPRESSION TAG	UNP P54998
B	-26	HIS	-	EXPRESSION TAG	UNP P54998
B	-25	SER	-	EXPRESSION TAG	UNP P54998
B	-24	SER	-	EXPRESSION TAG	UNP P54998
B	-23	GLY	-	EXPRESSION TAG	UNP P54998
B	-22	LEU	-	EXPRESSION TAG	UNP P54998
B	-21	VAL	-	EXPRESSION TAG	UNP P54998
B	-20	PRO	-	EXPRESSION TAG	UNP P54998
B	-19	ARG	-	EXPRESSION TAG	UNP P54998
B	-18	GLY	-	EXPRESSION TAG	UNP P54998
B	-17	SER	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP P54998
B	-15	MET	-	EXPRESSION TAG	UNP P54998
B	-14	ALA	-	EXPRESSION TAG	UNP P54998
B	-13	SER	-	EXPRESSION TAG	UNP P54998
B	-12	MET	-	EXPRESSION TAG	UNP P54998
B	-11	THR	-	EXPRESSION TAG	UNP P54998
B	-10	GLY	-	EXPRESSION TAG	UNP P54998
B	-9	GLY	-	EXPRESSION TAG	UNP P54998
B	-8	GLN	-	EXPRESSION TAG	UNP P54998
B	-7	GLN	-	EXPRESSION TAG	UNP P54998
B	-6	MET	-	EXPRESSION TAG	UNP P54998
B	-5	GLY	-	EXPRESSION TAG	UNP P54998
B	-4	ARG	-	EXPRESSION TAG	UNP P54998
B	-3	GLY	-	EXPRESSION TAG	UNP P54998
B	-2	SER	-	EXPRESSION TAG	UNP P54998
B	-1	GLU	-	EXPRESSION TAG	UNP P54998
B	0	PHE	-	EXPRESSION TAG	UNP P54998
C	-35	MET	-	EXPRESSION TAG	UNP P54998
C	-34	GLY	-	EXPRESSION TAG	UNP P54998
C	-33	SER	-	EXPRESSION TAG	UNP P54998
C	-32	SER	-	EXPRESSION TAG	UNP P54998
C	-31	HIS	-	EXPRESSION TAG	UNP P54998
C	-30	HIS	-	EXPRESSION TAG	UNP P54998
C	-29	HIS	-	EXPRESSION TAG	UNP P54998
C	-28	HIS	-	EXPRESSION TAG	UNP P54998
C	-27	HIS	-	EXPRESSION TAG	UNP P54998
C	-26	HIS	-	EXPRESSION TAG	UNP P54998
C	-25	SER	-	EXPRESSION TAG	UNP P54998
C	-24	SER	-	EXPRESSION TAG	UNP P54998
C	-23	GLY	-	EXPRESSION TAG	UNP P54998
C	-22	LEU	-	EXPRESSION TAG	UNP P54998
C	-21	VAL	-	EXPRESSION TAG	UNP P54998
C	-20	PRO	-	EXPRESSION TAG	UNP P54998
C	-19	ARG	-	EXPRESSION TAG	UNP P54998
C	-18	GLY	-	EXPRESSION TAG	UNP P54998
C	-17	SER	-	EXPRESSION TAG	UNP P54998
C	-16	HIS	-	EXPRESSION TAG	UNP P54998
C	-15	MET	-	EXPRESSION TAG	UNP P54998
C	-14	ALA	-	EXPRESSION TAG	UNP P54998
C	-13	SER	-	EXPRESSION TAG	UNP P54998
C	-12	MET	-	EXPRESSION TAG	UNP P54998
C	-11	THR	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	GLY	-	EXPRESSION TAG	UNP P54998
C	-9	GLY	-	EXPRESSION TAG	UNP P54998
C	-8	GLN	-	EXPRESSION TAG	UNP P54998
C	-7	GLN	-	EXPRESSION TAG	UNP P54998
C	-6	MET	-	EXPRESSION TAG	UNP P54998
C	-5	GLY	-	EXPRESSION TAG	UNP P54998
C	-4	ARG	-	EXPRESSION TAG	UNP P54998
C	-3	GLY	-	EXPRESSION TAG	UNP P54998
C	-2	SER	-	EXPRESSION TAG	UNP P54998
C	-1	GLU	-	EXPRESSION TAG	UNP P54998
C	0	PHE	-	EXPRESSION TAG	UNP P54998
D	-35	MET	-	EXPRESSION TAG	UNP P54998
D	-34	GLY	-	EXPRESSION TAG	UNP P54998
D	-33	SER	-	EXPRESSION TAG	UNP P54998
D	-32	SER	-	EXPRESSION TAG	UNP P54998
D	-31	HIS	-	EXPRESSION TAG	UNP P54998
D	-30	HIS	-	EXPRESSION TAG	UNP P54998
D	-29	HIS	-	EXPRESSION TAG	UNP P54998
D	-28	HIS	-	EXPRESSION TAG	UNP P54998
D	-27	HIS	-	EXPRESSION TAG	UNP P54998
D	-26	HIS	-	EXPRESSION TAG	UNP P54998
D	-25	SER	-	EXPRESSION TAG	UNP P54998
D	-24	SER	-	EXPRESSION TAG	UNP P54998
D	-23	GLY	-	EXPRESSION TAG	UNP P54998
D	-22	LEU	-	EXPRESSION TAG	UNP P54998
D	-21	VAL	-	EXPRESSION TAG	UNP P54998
D	-20	PRO	-	EXPRESSION TAG	UNP P54998
D	-19	ARG	-	EXPRESSION TAG	UNP P54998
D	-18	GLY	-	EXPRESSION TAG	UNP P54998
D	-17	SER	-	EXPRESSION TAG	UNP P54998
D	-16	HIS	-	EXPRESSION TAG	UNP P54998
D	-15	MET	-	EXPRESSION TAG	UNP P54998
D	-14	ALA	-	EXPRESSION TAG	UNP P54998
D	-13	SER	-	EXPRESSION TAG	UNP P54998
D	-12	MET	-	EXPRESSION TAG	UNP P54998
D	-11	THR	-	EXPRESSION TAG	UNP P54998
D	-10	GLY	-	EXPRESSION TAG	UNP P54998
D	-9	GLY	-	EXPRESSION TAG	UNP P54998
D	-8	GLN	-	EXPRESSION TAG	UNP P54998
D	-7	GLN	-	EXPRESSION TAG	UNP P54998
D	-6	MET	-	EXPRESSION TAG	UNP P54998
D	-5	GLY	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ARG	-	EXPRESSION TAG	UNP P54998
D	-3	GLY	-	EXPRESSION TAG	UNP P54998
D	-2	SER	-	EXPRESSION TAG	UNP P54998
D	-1	GLU	-	EXPRESSION TAG	UNP P54998
D	0	PHE	-	EXPRESSION TAG	UNP P54998
E	-35	MET	-	EXPRESSION TAG	UNP P54998
E	-34	GLY	-	EXPRESSION TAG	UNP P54998
E	-33	SER	-	EXPRESSION TAG	UNP P54998
E	-32	SER	-	EXPRESSION TAG	UNP P54998
E	-31	HIS	-	EXPRESSION TAG	UNP P54998
E	-30	HIS	-	EXPRESSION TAG	UNP P54998
E	-29	HIS	-	EXPRESSION TAG	UNP P54998
E	-28	HIS	-	EXPRESSION TAG	UNP P54998
E	-27	HIS	-	EXPRESSION TAG	UNP P54998
E	-26	HIS	-	EXPRESSION TAG	UNP P54998
E	-25	SER	-	EXPRESSION TAG	UNP P54998
E	-24	SER	-	EXPRESSION TAG	UNP P54998
E	-23	GLY	-	EXPRESSION TAG	UNP P54998
E	-22	LEU	-	EXPRESSION TAG	UNP P54998
E	-21	VAL	-	EXPRESSION TAG	UNP P54998
E	-20	PRO	-	EXPRESSION TAG	UNP P54998
E	-19	ARG	-	EXPRESSION TAG	UNP P54998
E	-18	GLY	-	EXPRESSION TAG	UNP P54998
E	-17	SER	-	EXPRESSION TAG	UNP P54998
E	-16	HIS	-	EXPRESSION TAG	UNP P54998
E	-15	MET	-	EXPRESSION TAG	UNP P54998
E	-14	ALA	-	EXPRESSION TAG	UNP P54998
E	-13	SER	-	EXPRESSION TAG	UNP P54998
E	-12	MET	-	EXPRESSION TAG	UNP P54998
E	-11	THR	-	EXPRESSION TAG	UNP P54998
E	-10	GLY	-	EXPRESSION TAG	UNP P54998
E	-9	GLY	-	EXPRESSION TAG	UNP P54998
E	-8	GLN	-	EXPRESSION TAG	UNP P54998
E	-7	GLN	-	EXPRESSION TAG	UNP P54998
E	-6	MET	-	EXPRESSION TAG	UNP P54998
E	-5	GLY	-	EXPRESSION TAG	UNP P54998
E	-4	ARG	-	EXPRESSION TAG	UNP P54998
E	-3	GLY	-	EXPRESSION TAG	UNP P54998
E	-2	SER	-	EXPRESSION TAG	UNP P54998
E	-1	GLU	-	EXPRESSION TAG	UNP P54998
E	0	PHE	-	EXPRESSION TAG	UNP P54998
F	-35	MET	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	-34	GLY	-	EXPRESSION TAG	UNP P54998
F	-33	SER	-	EXPRESSION TAG	UNP P54998
F	-32	SER	-	EXPRESSION TAG	UNP P54998
F	-31	HIS	-	EXPRESSION TAG	UNP P54998
F	-30	HIS	-	EXPRESSION TAG	UNP P54998
F	-29	HIS	-	EXPRESSION TAG	UNP P54998
F	-28	HIS	-	EXPRESSION TAG	UNP P54998
F	-27	HIS	-	EXPRESSION TAG	UNP P54998
F	-26	HIS	-	EXPRESSION TAG	UNP P54998
F	-25	SER	-	EXPRESSION TAG	UNP P54998
F	-24	SER	-	EXPRESSION TAG	UNP P54998
F	-23	GLY	-	EXPRESSION TAG	UNP P54998
F	-22	LEU	-	EXPRESSION TAG	UNP P54998
F	-21	VAL	-	EXPRESSION TAG	UNP P54998
F	-20	PRO	-	EXPRESSION TAG	UNP P54998
F	-19	ARG	-	EXPRESSION TAG	UNP P54998
F	-18	GLY	-	EXPRESSION TAG	UNP P54998
F	-17	SER	-	EXPRESSION TAG	UNP P54998
F	-16	HIS	-	EXPRESSION TAG	UNP P54998
F	-15	MET	-	EXPRESSION TAG	UNP P54998
F	-14	ALA	-	EXPRESSION TAG	UNP P54998
F	-13	SER	-	EXPRESSION TAG	UNP P54998
F	-12	MET	-	EXPRESSION TAG	UNP P54998
F	-11	THR	-	EXPRESSION TAG	UNP P54998
F	-10	GLY	-	EXPRESSION TAG	UNP P54998
F	-9	GLY	-	EXPRESSION TAG	UNP P54998
F	-8	GLN	-	EXPRESSION TAG	UNP P54998
F	-7	GLN	-	EXPRESSION TAG	UNP P54998
F	-6	MET	-	EXPRESSION TAG	UNP P54998
F	-5	GLY	-	EXPRESSION TAG	UNP P54998
F	-4	ARG	-	EXPRESSION TAG	UNP P54998
F	-3	GLY	-	EXPRESSION TAG	UNP P54998
F	-2	SER	-	EXPRESSION TAG	UNP P54998
F	-1	GLU	-	EXPRESSION TAG	UNP P54998
F	0	PHE	-	EXPRESSION TAG	UNP P54998
G	-35	MET	-	EXPRESSION TAG	UNP P54998
G	-34	GLY	-	EXPRESSION TAG	UNP P54998
G	-33	SER	-	EXPRESSION TAG	UNP P54998
G	-32	SER	-	EXPRESSION TAG	UNP P54998
G	-31	HIS	-	EXPRESSION TAG	UNP P54998
G	-30	HIS	-	EXPRESSION TAG	UNP P54998
G	-29	HIS	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	-28	HIS	-	EXPRESSION TAG	UNP P54998
G	-27	HIS	-	EXPRESSION TAG	UNP P54998
G	-26	HIS	-	EXPRESSION TAG	UNP P54998
G	-25	SER	-	EXPRESSION TAG	UNP P54998
G	-24	SER	-	EXPRESSION TAG	UNP P54998
G	-23	GLY	-	EXPRESSION TAG	UNP P54998
G	-22	LEU	-	EXPRESSION TAG	UNP P54998
G	-21	VAL	-	EXPRESSION TAG	UNP P54998
G	-20	PRO	-	EXPRESSION TAG	UNP P54998
G	-19	ARG	-	EXPRESSION TAG	UNP P54998
G	-18	GLY	-	EXPRESSION TAG	UNP P54998
G	-17	SER	-	EXPRESSION TAG	UNP P54998
G	-16	HIS	-	EXPRESSION TAG	UNP P54998
G	-15	MET	-	EXPRESSION TAG	UNP P54998
G	-14	ALA	-	EXPRESSION TAG	UNP P54998
G	-13	SER	-	EXPRESSION TAG	UNP P54998
G	-12	MET	-	EXPRESSION TAG	UNP P54998
G	-11	THR	-	EXPRESSION TAG	UNP P54998
G	-10	GLY	-	EXPRESSION TAG	UNP P54998
G	-9	GLY	-	EXPRESSION TAG	UNP P54998
G	-8	GLN	-	EXPRESSION TAG	UNP P54998
G	-7	GLN	-	EXPRESSION TAG	UNP P54998
G	-6	MET	-	EXPRESSION TAG	UNP P54998
G	-5	GLY	-	EXPRESSION TAG	UNP P54998
G	-4	ARG	-	EXPRESSION TAG	UNP P54998
G	-3	GLY	-	EXPRESSION TAG	UNP P54998
G	-2	SER	-	EXPRESSION TAG	UNP P54998
G	-1	GLU	-	EXPRESSION TAG	UNP P54998
G	0	PHE	-	EXPRESSION TAG	UNP P54998
H	-35	MET	-	EXPRESSION TAG	UNP P54998
H	-34	GLY	-	EXPRESSION TAG	UNP P54998
H	-33	SER	-	EXPRESSION TAG	UNP P54998
H	-32	SER	-	EXPRESSION TAG	UNP P54998
H	-31	HIS	-	EXPRESSION TAG	UNP P54998
H	-30	HIS	-	EXPRESSION TAG	UNP P54998
H	-29	HIS	-	EXPRESSION TAG	UNP P54998
H	-28	HIS	-	EXPRESSION TAG	UNP P54998
H	-27	HIS	-	EXPRESSION TAG	UNP P54998
H	-26	HIS	-	EXPRESSION TAG	UNP P54998
H	-25	SER	-	EXPRESSION TAG	UNP P54998
H	-24	SER	-	EXPRESSION TAG	UNP P54998
H	-23	GLY	-	EXPRESSION TAG	UNP P54998

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	-22	LEU	-	EXPRESSION TAG	UNP P54998
H	-21	VAL	-	EXPRESSION TAG	UNP P54998
H	-20	PRO	-	EXPRESSION TAG	UNP P54998
H	-19	ARG	-	EXPRESSION TAG	UNP P54998
H	-18	GLY	-	EXPRESSION TAG	UNP P54998
H	-17	SER	-	EXPRESSION TAG	UNP P54998
H	-16	HIS	-	EXPRESSION TAG	UNP P54998
H	-15	MET	-	EXPRESSION TAG	UNP P54998
H	-14	ALA	-	EXPRESSION TAG	UNP P54998
H	-13	SER	-	EXPRESSION TAG	UNP P54998
H	-12	MET	-	EXPRESSION TAG	UNP P54998
H	-11	THR	-	EXPRESSION TAG	UNP P54998
H	-10	GLY	-	EXPRESSION TAG	UNP P54998
H	-9	GLY	-	EXPRESSION TAG	UNP P54998
H	-8	GLN	-	EXPRESSION TAG	UNP P54998
H	-7	GLN	-	EXPRESSION TAG	UNP P54998
H	-6	MET	-	EXPRESSION TAG	UNP P54998
H	-5	GLY	-	EXPRESSION TAG	UNP P54998
H	-4	ARG	-	EXPRESSION TAG	UNP P54998
H	-3	GLY	-	EXPRESSION TAG	UNP P54998
H	-2	SER	-	EXPRESSION TAG	UNP P54998
H	-1	GLU	-	EXPRESSION TAG	UNP P54998
H	0	PHE	-	EXPRESSION TAG	UNP P54998

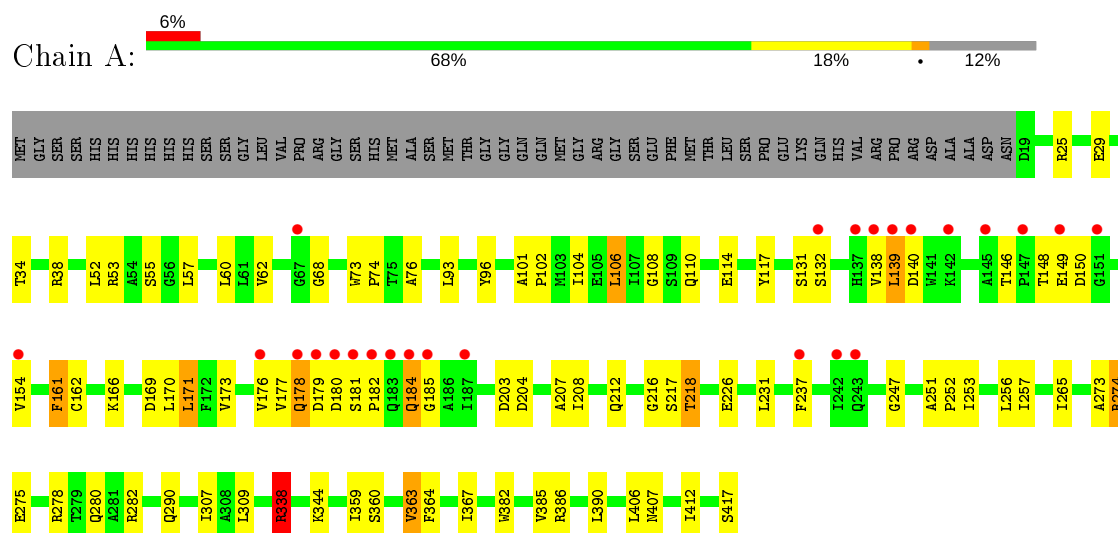
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	82	Total O 82 82	0	0
2	B	57	Total O 57 57	0	0
2	C	74	Total O 74 74	0	0
2	D	70	Total O 70 70	0	0
2	E	69	Total O 69 69	0	0
2	F	65	Total O 65 65	0	0
2	G	72	Total O 72 72	0	0
2	H	81	Total O 81 81	0	0

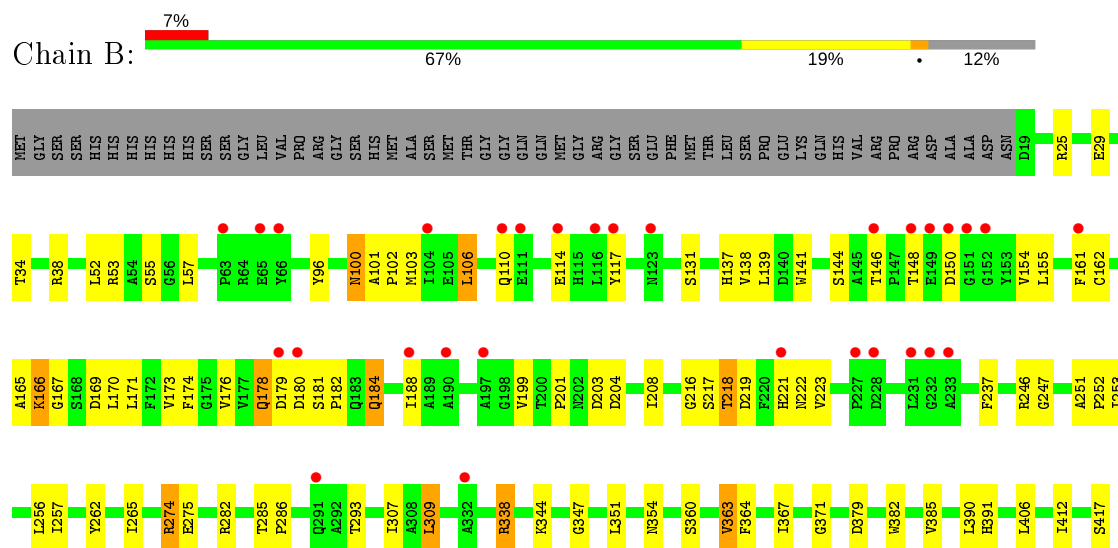
### 3 Residue-property plots

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.

#### • Molecule 1: Dibenzothiophene desulfurization enzyme C

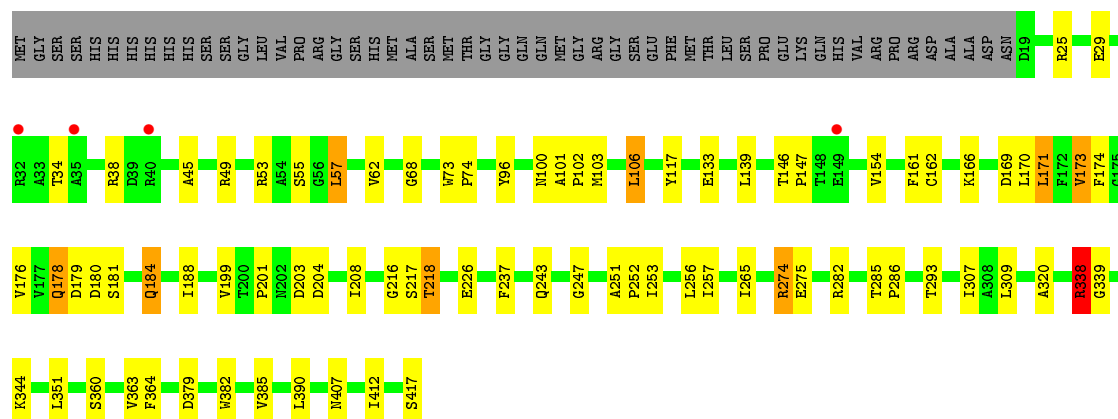


#### • Molecule 1: Dibenzothiophene desulfurization enzyme C

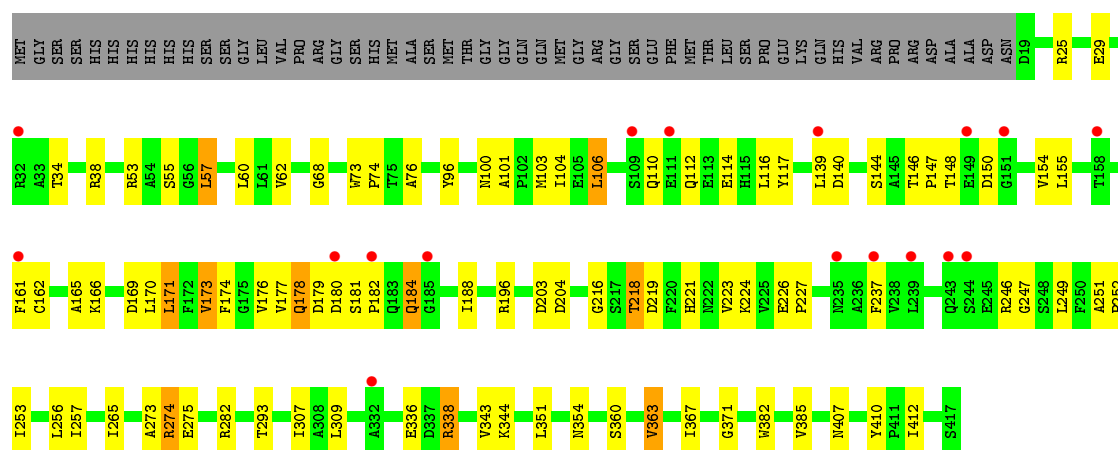


#### • Molecule 1: Dibenzothiophene desulfurization enzyme C

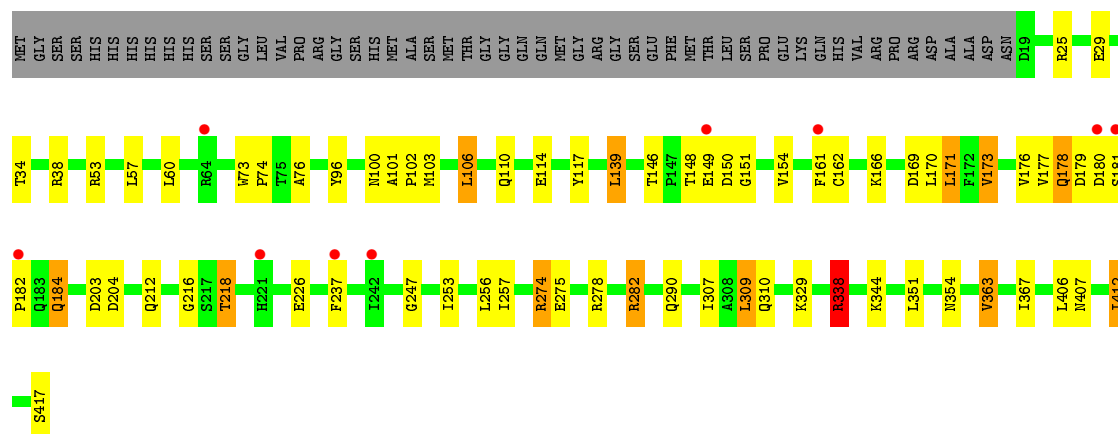
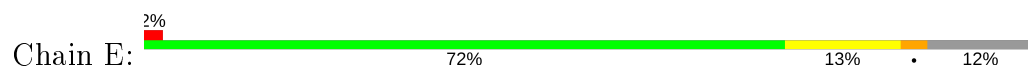




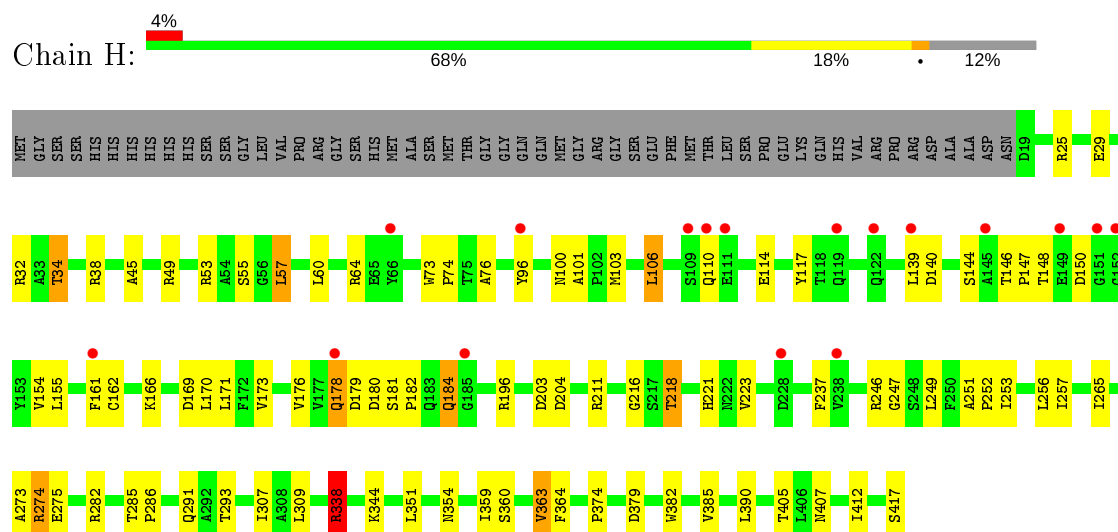
• Molecule 1: Dibenzothiophene desulfurization enzyme C



• Molecule 1: Dibenzothiophene desulfurization enzyme C



• Molecule 1: Dibenzothiophene desulfurization enzyme C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.16Å 96.27Å 98.56Å 81.03° 67.57° 85.84°	Depositor
Resolution (Å)	40.00 – 2.40 40.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.00-2.40) 96.2 (40.51-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.207 , 0.246 0.204 , 0.239	Depositor DCC
$R_{free}$ test set	3843 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.70	0/3116	0.69	2/4248 (0.0%)
1	B	0.71	2/3116 (0.1%)	0.65	0/4248
1	C	0.69	0/3116	0.69	2/4248 (0.0%)
1	D	0.71	1/3116 (0.0%)	0.66	1/4248 (0.0%)
1	E	0.68	0/3116	0.67	2/4248 (0.0%)
1	F	0.69	0/3116	0.65	0/4248
1	G	0.70	0/3116	0.68	2/4248 (0.0%)
1	H	0.68	0/3116	0.65	1/4248 (0.0%)
All	All	0.69	3/24928 (0.0%)	0.67	10/33984 (0.0%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	2
1	H	0	2
All	All	0	15

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ASN	CG-ND2	-6.60	1.16	1.32
1	B	100	ASN	CG-OD1	-6.48	1.09	1.24
1	D	343	VAL	CB-CG1	6.26	1.66	1.52



All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	338	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	C	338	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	C	338	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	G	338	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	G	338	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	338	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	338	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	H	338	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	E	338	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	338	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLN	Peptide
1	A	203	ASP	Peptide
1	B	178	GLN	Peptide
1	B	203	ASP	Peptide
1	C	178	GLN	Peptide
1	C	203	ASP	Peptide
1	D	178	GLN	Peptide
1	D	203	ASP	Peptide
1	E	178	GLN	Peptide
1	E	203	ASP	Peptide
1	F	203	ASP	Peptide
1	G	178	GLN	Peptide
1	G	203	ASP	Peptide
1	H	178	GLN	Peptide
1	H	203	ASP	Peptide

## 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	3041	0	2918	66	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3041	0	2918	63	2
1	C	3041	0	2918	43	5
1	D	3041	0	2918	62	0
1	E	3041	0	2918	41	3
1	F	3041	0	2918	52	2
1	G	3041	0	2918	48	1
1	H	3041	0	2918	67	0
2	A	82	0	0	15	0
2	B	57	0	0	7	0
2	C	74	0	0	3	0
2	D	70	0	0	12	0
2	E	69	0	0	4	0
2	F	65	0	0	3	0
2	G	72	0	0	6	0
2	H	81	0	0	12	0
All	All	24898	0	23344	395	10

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 (395) 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:H:223:VAL:HG13	2:H:561:HOH:O	1.37	1.20
1:G:302:TYR:HB3	2:G:542:HOH:O	1.42	1.17
1:B:137:HIS:CD2	1:H:221:HIS:CD2	2.35	1.15
1:A:139:LEU:HD11	2:A:537:HOH:O	1.62	0.98
1:A:139:LEU:HD13	2:A:539:HOH:O	1.66	0.96
1:F:161:PHE:HE1	2:G:532:HOH:O	1.50	0.94
1:D:180:ASP:H	1:D:184:GLN:HG3	1.32	0.93
1:H:354:ASN:HB2	2:H:506:HOH:O	1.69	0.92
1:A:138:VAL:HG23	2:A:539:HOH:O	1.69	0.91
2:G:542:HOH:O	1:H:405:THR:HB	1.71	0.91
1:A:180:ASP:H	1:A:184:GLN:HG3	1.34	0.90
1:F:180:ASP:H	1:F:184:GLN:HG3	1.37	0.89
1:C:180:ASP:H	1:C:184:GLN:HG3	1.37	0.89
1:E:180:ASP:H	1:E:184:GLN:HG3	1.37	0.89
1:B:180:ASP:H	1:B:184:GLN:HG3	1.38	0.87
1:H:180:ASP:H	1:H:184:GLN:HG3	1.39	0.87
1:G:180:ASP:H	1:G:184:GLN:HG3	1.39	0.86
1:B:137:HIS:CD2	1:H:221:HIS:HD2	1.92	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLN:HB3	2:D:562:HOH:O	1.77	0.83
1:E:282:ARG:NH1	2:E:562:HOH:O	2.12	0.81
1:D:221:HIS:CD2	1:F:137:HIS:CD2	2.70	0.80
1:F:282:ARG:NH1	2:F:558:HOH:O	2.15	0.79
1:D:224:LYS:O	2:D:557:HOH:O	2.01	0.78
1:F:44:SER:HB3	2:F:540:HOH:O	1.84	0.78
1:H:196:ARG:HD2	2:H:561:HOH:O	1.83	0.77
1:A:185:GLY:HA2	2:A:539:HOH:O	1.83	0.77
1:A:231:LEU:HB3	2:A:555:HOH:O	1.85	0.75
1:D:219:ASP:HB3	2:D:539:HOH:O	1.87	0.73
1:C:162:CYS:SG	1:C:218:THR:HG23	2.29	0.73
1:D:410:TYR:CZ	2:D:554:HOH:O	2.42	0.73
1:F:162:CYS:SG	1:F:218:THR:HG23	2.29	0.72
1:C:106:LEU:HG	1:C:247:GLY:HA2	1.71	0.72
1:D:104:ILE:HG23	2:D:562:HOH:O	1.89	0.72
1:B:137:HIS:CG	1:H:221:HIS:CD2	2.77	0.72
1:B:166:LYS:HB3	2:B:547:HOH:O	1.88	0.71
1:C:133:GLU:OE1	2:C:561:HOH:O	2.07	0.71
1:H:196:ARG:CD	2:H:561:HOH:O	2.40	0.70
1:H:196:ARG:HG2	2:H:561:HOH:O	1.91	0.69
1:B:162:CYS:SG	1:B:218:THR:HG23	2.33	0.69
1:E:162:CYS:SG	1:E:218:THR:HG23	2.33	0.68
1:D:336:GLU:HA	2:D:554:HOH:O	1.92	0.68
1:B:219:ASP:OD2	2:B:540:HOH:O	2.12	0.68
1:H:196:ARG:CG	2:H:561:HOH:O	2.41	0.68
1:H:291:GLN:OE1	2:H:524:HOH:O	2.12	0.67
1:F:379:ASP:HB3	1:G:208:ILE:HD13	1.75	0.67
1:A:162:CYS:SG	1:A:218:THR:HG23	2.35	0.66
1:A:231:LEU:HD22	2:A:555:HOH:O	1.93	0.66
1:G:162:CYS:SG	1:G:218:THR:HG23	2.35	0.66
1:E:106:LEU:HG	1:E:247:GLY:HA2	1.79	0.65
1:A:180:ASP:N	1:A:184:GLN:HG3	2.08	0.65
1:B:167:GLY:N	2:B:547:HOH:O	2.30	0.65
1:D:106:LEU:HG	1:D:247:GLY:HA2	1.79	0.65
1:A:280:GLN:HG3	2:A:568:HOH:O	1.98	0.64
1:A:146:THR:HB	1:A:154:VAL:HG23	1.79	0.63
1:F:106:LEU:HG	1:F:247:GLY:HA2	1.80	0.63
1:D:410:TYR:CE1	2:D:554:HOH:O	2.49	0.63
1:H:253:ILE:O	1:H:257:ILE:HG12	2.00	0.62
1:E:180:ASP:N	1:E:184:GLN:HG3	2.12	0.62
1:D:53:ARG:NH2	1:D:169:ASP:OD2	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:HIS:CG	1:H:221:HIS:NE2	2.67	0.62
1:E:53:ARG:NH2	1:E:169:ASP:OD2	2.33	0.62
1:G:375:ARG:HD3	2:G:550:HOH:O	1.99	0.62
1:D:180:ASP:N	1:D:184:GLN:HG3	2.09	0.61
1:C:204:ASP:OD2	1:C:217:SER:OG	2.16	0.61
1:H:106:LEU:HG	1:H:247:GLY:HA2	1.81	0.61
1:B:106:LEU:HG	1:B:247:GLY:HA2	1.82	0.61
1:G:407:ASN:OD1	1:H:293:THR:HB	2.01	0.61
1:E:329:LYS:HE3	2:E:559:HOH:O	2.00	0.61
1:A:140:ASP:HB2	2:A:501:HOH:O	2.01	0.60
1:F:180:ASP:N	1:F:184:GLN:HG3	2.12	0.60
1:E:290:GLN:NE2	1:H:140:ASP:OD2	2.35	0.60
1:A:53:ARG:NH2	1:A:169:ASP:OD2	2.35	0.59
1:G:53:ARG:NH2	1:G:169:ASP:OD2	2.35	0.59
1:A:108:GLY:CA	2:A:555:HOH:O	2.49	0.59
1:B:354:ASN:HB2	2:B:542:HOH:O	2.02	0.59
1:A:140:ASP:CB	2:A:501:HOH:O	2.51	0.59
1:C:53:ARG:NH2	1:C:169:ASP:OD2	2.35	0.59
1:C:180:ASP:N	1:C:184:GLN:HG3	2.14	0.58
1:B:34:THR:OG1	1:B:38:ARG:NH1	2.36	0.58
1:B:379:ASP:HB3	1:C:208:ILE:HD13	1.86	0.58
1:A:106:LEU:HG	1:A:247:GLY:HA2	1.86	0.58
1:A:204:ASP:OD2	1:A:217:SER:OG	2.15	0.58
1:D:196:ARG:HD2	2:D:557:HOH:O	2.03	0.57
1:B:137:HIS:CB	1:H:221:HIS:NE2	2.67	0.57
1:F:339:GLY:HA2	2:F:512:HOH:O	2.04	0.57
1:F:204:ASP:HB3	1:F:216:GLY:HA3	1.86	0.57
1:G:204:ASP:HB3	1:G:216:GLY:HA3	1.86	0.57
1:B:180:ASP:N	1:B:184:GLN:HG3	2.14	0.57
1:F:274:ARG:HG3	1:F:275:GLU:N	2.18	0.57
1:F:364:PHE:HB3	1:G:390:LEU:HD11	1.86	0.57
1:B:293:THR:HB	1:E:407:ASN:OD1	2.04	0.57
1:H:180:ASP:N	1:H:184:GLN:HG3	2.14	0.57
1:G:180:ASP:N	1:G:184:GLN:HG3	2.17	0.57
1:B:364:PHE:HB3	1:C:390:LEU:HD11	1.87	0.56
1:D:146:THR:HB	1:D:154:VAL:HG23	1.87	0.56
1:G:106:LEU:HG	1:G:247:GLY:HA2	1.87	0.56
1:B:406:LEU:O	1:E:278:ARG:HD2	2.06	0.56
1:E:146:THR:HB	1:E:154:VAL:HG23	1.88	0.56
1:B:347:GLY:HA3	1:E:310:GLN:OE1	2.05	0.56
1:H:162:CYS:SG	1:H:218:THR:HG23	2.46	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:265:ILE:HG21	1:G:385:VAL:HG23	1.88	0.55
1:D:34:THR:OG1	1:D:38:ARG:NH1	2.40	0.55
1:G:285:THR:N	1:G:286:PRO:CD	2.70	0.55
1:A:34:THR:OG1	1:A:38:ARG:NH1	2.40	0.55
1:B:204:ASP:HB3	1:B:216:GLY:HA3	1.89	0.55
1:G:293:THR:HB	1:H:407:ASN:OD1	2.07	0.55
1:B:253:ILE:O	1:B:257:ILE:HG12	2.07	0.55
1:C:34:THR:OG1	1:C:38:ARG:NH1	2.40	0.55
1:D:253:ILE:O	1:D:257:ILE:HG12	2.08	0.54
1:D:274:ARG:HG3	1:D:275:GLU:N	2.21	0.54
1:B:137:HIS:HB2	1:H:221:HIS:NE2	2.22	0.54
1:C:204:ASP:HB3	1:C:216:GLY:HA3	1.89	0.54
1:F:208:ILE:HD13	1:G:379:ASP:HB3	1.90	0.54
1:C:45:ALA:O	1:C:49:ARG:HG3	2.08	0.54
1:F:253:ILE:O	1:F:257:ILE:HG12	2.08	0.54
1:B:176:VAL:O	1:B:178:GLN:HG3	2.07	0.54
1:E:176:VAL:O	1:E:178:GLN:HG3	2.08	0.54
1:F:34:THR:OG1	1:F:38:ARG:NH1	2.42	0.53
1:F:390:LEU:HD11	1:G:364:PHE:HB3	1.90	0.53
1:D:162:CYS:SG	1:D:218:THR:HG23	2.48	0.53
1:D:176:VAL:O	1:D:178:GLN:HG3	2.08	0.53
1:A:274:ARG:HG3	1:A:275:GLU:N	2.24	0.53
1:E:253:ILE:O	1:E:257:ILE:HG12	2.09	0.52
1:G:34:THR:OG1	1:G:38:ARG:NH1	2.42	0.52
1:H:146:THR:HB	1:H:154:VAL:HG23	1.91	0.52
1:A:52:LEU:O	1:A:55:SER:OG	2.25	0.52
1:B:274:ARG:HG3	1:B:275:GLU:N	2.24	0.52
1:C:253:ILE:O	1:C:257:ILE:HG12	2.09	0.52
1:D:116:LEU:HD12	2:D:562:HOH:O	2.08	0.52
1:D:265:ILE:HG21	1:D:385:VAL:HG23	1.90	0.52
1:F:204:ASP:OD2	1:F:217:SER:OG	2.17	0.52
1:H:34:THR:OG1	1:H:38:ARG:NH1	2.42	0.52
1:F:53:ARG:NH2	1:F:169:ASP:OD2	2.43	0.52
1:F:176:VAL:O	1:F:178:GLN:HG3	2.10	0.52
1:G:370:ARG:HG3	2:G:532:HOH:O	2.09	0.51
1:H:32:ARG:HD3	2:H:547:HOH:O	2.09	0.51
1:G:176:VAL:O	1:G:178:GLN:HG3	2.11	0.51
1:H:32:ARG:NH1	2:H:547:HOH:O	2.21	0.51
1:D:204:ASP:HB3	1:D:216:GLY:HA3	1.91	0.51
1:E:274:ARG:HG3	1:E:275:GLU:N	2.26	0.51
1:D:148:THR:OG1	1:D:150:ASP:OD1	2.18	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:HIS:HB3	2:B:519:HOH:O	2.11	0.50
1:D:62:VAL:O	1:D:68:GLY:HA3	2.12	0.50
1:E:354:ASN:HB2	2:E:520:HOH:O	2.10	0.50
1:G:351:LEU:HG	1:H:307:ILE:HG23	1.93	0.50
1:H:53:ARG:NH2	1:H:169:ASP:OD2	2.44	0.50
1:F:148:THR:OG1	1:F:150:ASP:OD1	2.18	0.50
1:D:221:HIS:NE2	1:F:137:HIS:CG	2.80	0.50
1:C:55:SER:OG	1:C:57:LEU:HB2	2.12	0.50
1:H:265:ILE:HG21	1:H:385:VAL:HG23	1.92	0.50
1:B:165:ALA:HB3	2:B:513:HOH:O	2.12	0.50
1:B:101:ALA:HB1	1:B:117:TYR:HE1	1.77	0.50
1:H:204:ASP:HB3	1:H:216:GLY:HA3	1.93	0.49
1:A:131:SER:OG	1:A:132:SER:N	2.41	0.49
1:B:360:SER:HB3	1:B:382:TRP:HB2	1.94	0.49
1:H:211:ARG:HD2	2:H:541:HOH:O	2.11	0.49
1:D:110:GLN:O	1:D:114:GLU:HG3	2.12	0.49
1:B:390:LEU:HD11	1:C:364:PHE:HB3	1.93	0.49
1:B:165:ALA:N	2:B:513:HOH:O	2.43	0.49
1:C:179:ASP:HB3	1:C:181:SER:HB2	1.95	0.49
1:C:320:ALA:HB2	2:C:535:HOH:O	2.12	0.49
1:F:146:THR:HB	1:F:154:VAL:HG23	1.94	0.49
1:G:307:ILE:HG23	1:H:351:LEU:HG	1.94	0.49
1:D:101:ALA:HB1	1:D:117:TYR:HE1	1.76	0.48
1:B:146:THR:HB	1:B:154:VAL:HG23	1.94	0.48
1:A:407:ASN:OD1	1:F:293:THR:HB	2.12	0.48
1:G:360:SER:HB3	1:G:382:TRP:HB2	1.95	0.48
1:H:338:ARG:NH2	1:H:417:SER:O	2.45	0.48
1:F:179:ASP:O	1:F:180:ASP:HB2	2.13	0.48
1:H:179:ASP:HB3	1:H:181:SER:H	1.79	0.48
1:B:179:ASP:O	1:B:180:ASP:HB2	2.13	0.48
1:C:146:THR:HB	1:C:154:VAL:HG23	1.95	0.48
1:G:45:ALA:O	1:G:49:ARG:HG3	2.14	0.48
1:H:223:VAL:CG1	2:H:561:HOH:O	2.21	0.48
1:H:249:LEU:C	1:H:252:PRO:HD2	2.34	0.48
1:H:360:SER:HB3	1:H:382:TRP:HB2	1.95	0.48
1:C:293:THR:HB	1:D:407:ASN:OD1	2.14	0.48
1:B:293:THR:HA	1:E:406:LEU:HD21	1.95	0.48
1:E:101:ALA:HB1	1:E:117:TYR:HE1	1.79	0.48
1:A:406:LEU:HD21	1:F:293:THR:HA	1.96	0.48
1:A:138:VAL:CG2	2:A:539:HOH:O	2.45	0.48
1:D:354:ASN:HB2	2:D:507:HOH:O	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ARG:NH2	1:F:417:SER:O	2.44	0.48
1:H:176:VAL:O	1:H:178:GLN:HG3	2.14	0.48
1:A:204:ASP:HB3	1:A:216:GLY:HA3	1.94	0.47
1:E:73:TRP:HB2	1:E:74:PRO:HD3	1.96	0.47
1:H:148:THR:OG1	1:H:150:ASP:OD1	2.22	0.47
1:F:131:SER:HB2	1:F:174:PHE:CE1	2.49	0.47
1:A:208:ILE:HD13	1:H:379:ASP:HB3	1.97	0.47
1:A:338:ARG:NH2	1:A:417:SER:O	2.48	0.47
1:G:146:THR:HB	1:G:154:VAL:HG23	1.96	0.47
1:A:265:ILE:HG21	1:A:385:VAL:HG23	1.97	0.47
1:H:251:ALA:N	1:H:252:PRO:CD	2.78	0.47
1:D:179:ASP:HB3	1:D:181:SER:H	1.80	0.47
1:G:179:ASP:HB3	1:G:181:SER:HB2	1.97	0.47
1:C:285:THR:N	1:C:286:PRO:CD	2.78	0.47
1:H:60:LEU:HD21	1:H:76:ALA:HA	1.96	0.47
1:A:101:ALA:O	1:A:104:ILE:HB	2.15	0.47
1:E:354:ASN:HB2	2:E:549:HOH:O	2.14	0.47
1:F:45:ALA:O	1:F:49:ARG:HG3	2.15	0.47
1:A:171:LEU:HD13	1:A:173:VAL:HG22	1.97	0.47
1:B:221:HIS:H	1:B:223:VAL:HG23	1.80	0.47
1:C:179:ASP:O	1:C:180:ASP:HB2	2.14	0.47
1:H:73:TRP:HB2	1:H:74:PRO:HD3	1.97	0.47
1:B:179:ASP:HB3	1:B:181:SER:H	1.80	0.46
1:D:221:HIS:NE2	1:F:137:HIS:CB	2.78	0.46
1:A:253:ILE:O	1:A:257:ILE:HG12	2.15	0.46
1:B:181:SER:OG	1:B:182:PRO:HD2	2.14	0.46
1:C:265:ILE:HG21	1:C:385:VAL:HG23	1.97	0.46
1:F:179:ASP:HB3	1:F:181:SER:H	1.81	0.46
1:G:156:ASN:ND2	2:G:549:HOH:O	1.80	0.46
1:H:179:ASP:HB3	1:H:181:SER:HB2	1.97	0.46
1:B:100:ASN:O	1:B:103:MET:HB3	2.15	0.46
1:D:171:LEU:HD13	1:D:173:VAL:HG22	1.98	0.46
1:C:274:ARG:HG3	1:C:275:GLU:N	2.31	0.46
1:G:179:ASP:O	1:G:180:ASP:HB2	2.15	0.46
1:G:62:VAL:O	1:G:68:GLY:HA3	2.16	0.46
1:C:179:ASP:HB3	1:C:181:SER:H	1.80	0.46
1:A:307:ILE:HG23	1:F:351:LEU:HG	1.97	0.46
1:D:179:ASP:HB3	1:D:181:SER:HB2	1.98	0.46
1:E:60:LEU:HD21	1:E:76:ALA:HA	1.98	0.46
1:B:204:ASP:OD2	1:B:217:SER:OG	2.18	0.46
1:B:363:VAL:HG13	1:B:367:ILE:HD12	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:VAL:O	1:C:178:GLN:HG3	2.15	0.46
1:D:154:VAL:HA	1:D:223:VAL:O	2.16	0.46
1:A:108:GLY:HA3	2:A:555:HOH:O	2.14	0.46
1:H:273:ALA:CB	1:H:363:VAL:HG22	2.46	0.45
1:A:251:ALA:N	1:A:252:PRO:CD	2.79	0.45
1:D:360:SER:HB3	1:D:382:TRP:HB2	1.98	0.45
1:G:253:ILE:O	1:G:257:ILE:HG12	2.17	0.45
1:A:148:THR:OG1	1:A:150:ASP:OD1	2.19	0.45
1:A:290:GLN:NE2	1:D:140:ASP:OD2	2.49	0.45
1:C:101:ALA:N	1:C:102:PRO:CD	2.79	0.45
1:A:101:ALA:N	1:A:102:PRO:HD2	2.32	0.45
1:A:139:LEU:HA	1:A:139:LEU:HD12	1.78	0.45
1:F:179:ASP:HB3	1:F:181:SER:HB2	1.97	0.45
1:B:179:ASP:HB3	1:B:181:SER:HB2	1.99	0.45
1:D:249:LEU:C	1:D:252:PRO:HD2	2.37	0.45
1:E:179:ASP:HB3	1:E:181:SER:HB2	1.99	0.45
1:G:101:ALA:N	1:G:102:PRO:HD2	2.31	0.45
1:D:144:SER:O	1:D:155:LEU:HA	2.17	0.45
1:D:181:SER:OG	1:D:182:PRO:HD2	2.17	0.45
1:D:227:PRO:HA	2:D:560:HOH:O	2.16	0.45
1:D:73:TRP:HB2	1:D:74:PRO:HD3	1.99	0.45
1:B:208:ILE:HD13	1:C:379:ASP:HB3	1.99	0.45
1:D:179:ASP:O	1:D:180:ASP:HB2	2.17	0.45
1:E:204:ASP:HB3	1:E:216:GLY:HA3	1.97	0.45
1:C:101:ALA:HB1	1:C:117:TYR:HE1	1.82	0.44
1:D:221:HIS:NE2	1:F:137:HIS:HB2	2.31	0.44
1:D:106:LEU:HD12	1:D:246:ARG:HG2	1.99	0.44
1:E:363:VAL:HG13	1:E:367:ILE:HD12	1.99	0.44
1:H:100:ASN:O	1:H:103:MET:HB3	2.18	0.44
1:H:359:ILE:O	1:H:363:VAL:HB	2.17	0.44
1:H:45:ALA:O	1:H:49:ARG:HG3	2.17	0.44
1:A:179:ASP:O	1:A:180:ASP:HB2	2.17	0.44
1:B:338:ARG:NH2	1:B:417:SER:O	2.49	0.44
1:A:101:ALA:N	1:A:102:PRO:CD	2.81	0.44
1:A:140:ASP:HB3	2:A:501:HOH:O	2.15	0.44
1:F:106:LEU:HD12	1:F:246:ARG:HG2	2.00	0.44
1:G:338:ARG:NH2	1:G:417:SER:O	2.48	0.44
1:E:309:LEU:HA	1:E:309:LEU:HD12	1.88	0.44
1:G:174:PHE:HA	1:G:188:ILE:O	2.18	0.44
1:C:100:ASN:O	1:C:103:MET:HB3	2.18	0.44
1:D:273:ALA:CB	1:D:363:VAL:HG22	2.47	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:285:THR:N	1:F:286:PRO:CD	2.81	0.44
1:G:101:ALA:N	1:G:102:PRO:CD	2.80	0.44
1:G:148:THR:OG1	1:G:150:ASP:OD1	2.19	0.44
1:G:274:ARG:HG3	1:G:275:GLU:N	2.32	0.44
1:H:64:ARG:NH1	2:H:560:HOH:O	2.47	0.44
1:B:101:ALA:N	1:B:102:PRO:CD	2.81	0.44
1:C:360:SER:HB3	1:C:382:TRP:HB2	1.99	0.44
1:E:148:THR:OG1	1:E:150:ASP:OD1	2.18	0.44
1:F:100:ASN:O	1:F:103:MET:HB3	2.18	0.44
1:A:101:ALA:HB1	1:A:117:TYR:HE1	1.83	0.44
1:A:38:ARG:HB3	1:A:212:GLN:OE1	2.18	0.44
1:H:106:LEU:HD12	1:H:246:ARG:HG2	1.99	0.44
1:B:137:HIS:CD2	1:H:221:HIS:NE2	2.78	0.44
1:E:179:ASP:O	1:E:180:ASP:HB2	2.18	0.44
1:H:144:SER:O	1:H:155:LEU:HA	2.18	0.44
1:H:179:ASP:O	1:H:180:ASP:HB2	2.17	0.44
1:A:177:VAL:HG12	1:A:179:ASP:HB2	1.99	0.43
1:A:359:ILE:O	1:A:363:VAL:HB	2.18	0.43
1:A:60:LEU:HD21	1:A:76:ALA:HA	2.00	0.43
1:H:101:ALA:HB1	1:H:117:TYR:HE1	1.82	0.43
1:A:179:ASP:HB3	1:A:181:SER:HB2	2.00	0.43
1:C:171:LEU:HD13	1:C:173:VAL:HG22	1.99	0.43
1:F:181:SER:OG	1:F:182:PRO:HD2	2.17	0.43
1:B:251:ALA:N	1:B:252:PRO:CD	2.81	0.43
1:C:307:ILE:HG23	1:D:351:LEU:HG	2.00	0.43
1:E:38:ARG:HB3	1:E:212:GLN:OE1	2.18	0.43
1:C:407:ASN:OD1	1:D:293:THR:HB	2.19	0.43
1:E:171:LEU:HD13	1:E:173:VAL:HG22	2.01	0.43
1:G:406:LEU:HD21	1:H:293:THR:HA	2.00	0.43
1:A:364:PHE:HB3	1:H:390:LEU:HD11	2.00	0.43
1:B:363:VAL:HG13	1:B:367:ILE:CD1	2.49	0.43
1:C:174:PHE:HA	1:C:188:ILE:O	2.19	0.43
1:E:110:GLN:O	1:E:114:GLU:HG3	2.18	0.43
1:E:181:SER:OG	1:E:182:PRO:HD2	2.18	0.43
1:F:177:VAL:HG12	1:F:179:ASP:HB2	2.00	0.43
1:A:181:SER:OG	1:A:182:PRO:HD2	2.18	0.43
1:A:251:ALA:N	1:A:252:PRO:HD2	2.34	0.43
1:A:273:ALA:CB	1:A:363:VAL:HG22	2.49	0.43
1:D:101:ALA:O	1:D:104:ILE:HB	2.19	0.43
1:A:278:ARG:HD2	1:F:406:LEU:O	2.18	0.43
1:B:148:THR:OG1	1:B:150:ASP:OD1	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:HIS:CD2	1:F:137:HIS:CG	3.07	0.43
1:D:367:ILE:CG2	1:D:371:GLY:HA3	2.49	0.43
1:A:176:VAL:O	1:A:178:GLN:HG3	2.18	0.42
1:C:73:TRP:HB2	1:C:74:PRO:HD3	2.00	0.42
1:E:412:ILE:H	1:E:412:ILE:HG12	1.58	0.42
1:F:64:ARG:HA	1:F:68:GLY:O	2.19	0.42
1:H:181:SER:OG	1:H:182:PRO:HD2	2.18	0.42
1:E:34:THR:OG1	1:E:38:ARG:NH1	2.51	0.42
1:F:174:PHE:HA	1:F:188:ILE:O	2.19	0.42
1:F:374:PRO:HD3	1:G:207:ALA:HA	2.01	0.42
1:H:154:VAL:HA	1:H:223:VAL:O	2.19	0.42
1:H:274:ARG:HG3	1:H:275:GLU:N	2.34	0.42
1:B:53:ARG:NH2	1:B:169:ASP:OD2	2.51	0.42
1:C:338:ARG:NH2	1:C:417:SER:O	2.49	0.42
1:D:226:GLU:HA	1:D:226:GLU:OE1	2.19	0.42
1:B:199:VAL:HG12	1:B:201:PRO:HD3	2.01	0.42
1:B:285:THR:N	1:B:286:PRO:CD	2.83	0.42
1:F:360:SER:HB3	1:F:382:TRP:HB2	2.01	0.42
1:B:307:ILE:HG23	1:E:351:LEU:HG	2.00	0.42
1:C:251:ALA:N	1:C:252:PRO:CD	2.82	0.42
1:H:55:SER:OG	1:H:57:LEU:HB2	2.20	0.42
1:A:146:THR:HB	1:A:154:VAL:CG2	2.45	0.42
1:F:101:ALA:HB1	1:F:117:TYR:HE1	1.84	0.42
1:H:146:THR:HA	1:H:147:PRO:HD3	1.92	0.42
1:A:179:ASP:HB3	1:A:181:SER:H	1.82	0.42
1:F:249:LEU:C	1:F:252:PRO:HD2	2.40	0.42
1:A:108:GLY:N	2:A:555:HOH:O	2.53	0.42
1:D:106:LEU:HD12	1:D:106:LEU:HA	1.94	0.42
1:D:165:ALA:HB3	2:D:548:HOH:O	2.20	0.42
1:G:55:SER:OG	1:G:57:LEU:HB2	2.20	0.42
1:B:131:SER:HB2	1:B:174:PHE:CE1	2.55	0.42
1:G:159:LYS:HE2	1:G:159:LYS:HB2	1.91	0.42
1:D:146:THR:HA	1:D:147:PRO:HD3	1.94	0.42
1:H:285:THR:N	1:H:286:PRO:CD	2.83	0.42
1:C:351:LEU:HG	1:D:307:ILE:HG23	2.02	0.41
1:C:62:VAL:O	1:C:68:GLY:HA3	2.20	0.41
1:D:60:LEU:HD21	1:D:76:ALA:HA	2.02	0.41
1:F:101:ALA:N	1:F:102:PRO:CD	2.82	0.41
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.78	0.41
1:B:52:LEU:O	1:B:55:SER:OG	2.24	0.41
1:A:360:SER:HB3	1:A:382:TRP:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:THR:HA	1:C:147:PRO:HD3	1.92	0.41
1:D:55:SER:OG	1:D:57:LEU:HB2	2.21	0.41
1:G:73:TRP:HB2	1:G:74:PRO:HD3	2.02	0.41
1:A:110:GLN:O	1:A:114:GLU:HG3	2.20	0.41
1:A:386:ARG:HD3	1:H:364:PHE:CD1	2.54	0.41
1:B:367:ILE:CG2	1:B:371:GLY:HA3	2.50	0.41
1:F:57:LEU:HD12	1:F:57:LEU:HA	1.91	0.41
1:A:73:TRP:HB2	1:A:74:PRO:HD3	2.02	0.41
1:B:144:SER:O	1:B:155:LEU:HA	2.21	0.41
1:C:101:ALA:N	1:C:102:PRO:HD2	2.34	0.41
1:G:179:ASP:HB3	1:G:181:SER:H	1.85	0.41
1:H:249:LEU:HD23	1:H:249:LEU:HA	1.86	0.41
1:B:174:PHE:HA	1:B:188:ILE:O	2.21	0.41
1:B:262:TYR:CD1	1:B:262:TYR:N	2.89	0.41
1:B:351:LEU:HG	1:E:307:ILE:HG23	2.01	0.41
1:F:110:GLN:O	1:F:114:GLU:HG3	2.20	0.41
1:B:138:VAL:HA	1:B:141:TRP:CD1	2.55	0.41
1:E:179:ASP:HB3	1:E:181:SER:H	1.84	0.41
1:G:103:MET:HG3	1:G:237:PHE:HZ	1.86	0.41
1:D:363:VAL:HG13	1:D:367:ILE:CD1	2.50	0.41
1:E:100:ASN:O	1:E:103:MET:HB3	2.20	0.41
1:B:265:ILE:HG21	1:B:385:VAL:HG23	2.02	0.41
1:C:199:VAL:HG12	1:C:201:PRO:HD3	2.03	0.41
1:G:412:ILE:HG12	1:G:412:ILE:H	1.64	0.41
1:A:207:ALA:HA	1:H:374:PRO:HD3	2.03	0.41
1:A:363:VAL:HG13	1:A:367:ILE:HD12	2.02	0.41
1:D:174:PHE:HA	1:D:188:ILE:O	2.20	0.41
1:E:101:ALA:N	1:E:102:PRO:CD	2.84	0.41
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.87	0.41
1:C:339:GLY:HA2	2:C:567:HOH:O	2.21	0.41
1:G:248:SER:OG	1:G:338:ARG:HD3	2.21	0.40
1:A:161:PHE:O	2:A:514:HOH:O	2.22	0.40
1:B:106:LEU:HD12	1:B:246:ARG:HG2	2.04	0.40
1:D:100:ASN:O	1:D:103:MET:HB3	2.20	0.40
1:E:139:LEU:HA	1:E:139:LEU:HD12	1.94	0.40
1:A:390:LEU:HD11	1:H:364:PHE:HB3	2.02	0.40
1:E:177:VAL:HG12	1:E:179:ASP:HB2	2.02	0.40
1:G:100:ASN:O	1:G:103:MET:HB3	2.22	0.40
1:G:101:ALA:HB1	1:G:117:TYR:HE1	1.86	0.40
1:G:359:ILE:O	1:G:363:VAL:HB	2.21	0.40
1:H:110:GLN:O	1:H:114:GLU:HG3	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:GLN:O	1:B:114:GLU:HG3	2.21	0.40
1:G:251:ALA:N	1:G:252:PRO:CD	2.84	0.40
1:A:62:VAL:O	1:A:68:GLY:HA3	2.21	0.40
1:D:177:VAL:HG12	1:D:179:ASP:HB2	2.04	0.40
1:D:251:ALA:N	1:D:252:PRO:CD	2.85	0.40
1:E:338:ARG:NH2	1:E:417:SER:O	2.53	0.40
1:F:221:HIS:H	1:F:223:VAL:HG23	1.86	0.40
1:F:265:ILE:HG21	1:F:385:VAL:HG23	2.03	0.40

All (10) 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:C:226:GLU:OE2	1:E:226:GLU:OE2[1_565]	1.81	0.39
1:A:226:GLU:OE2	1:G:226:GLU:OE2[1_455]	1.84	0.36
1:A:140:ASP:OD2	1:C:243:GLN:NE2[1_546]	1.85	0.35
1:A:140:ASP:OD1	1:C:243:GLN:NE2[1_546]	1.92	0.28
1:E:149:GLU:O	1:F:222:ASN:ND2[1_455]	2.00	0.20
1:A:149:GLU:O	1:B:222:ASN:ND2[1_545]	2.03	0.17
1:A:140:ASP:OD2	1:C:243:GLN:CD[1_546]	2.07	0.13
1:E:151:GLY:CA	1:F:221:HIS:CE1[1_455]	2.09	0.11
1:A:140:ASP:CG	1:C:243:GLN:NE2[1_546]	2.10	0.10
1:A:150:ASP:O	1:B:221:HIS:NE2[1_545]	2.13	0.07

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/453 (88%)	388 (98%)	9 (2%)	0	100	100
1	B	397/453 (88%)	389 (98%)	8 (2%)	0	100	100
1	C	397/453 (88%)	391 (98%)	6 (2%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	397/453 (88%)	390 (98%)	7 (2%)	0	100	100
1	E	397/453 (88%)	388 (98%)	9 (2%)	0	100	100
1	F	397/453 (88%)	392 (99%)	5 (1%)	0	100	100
1	G	397/453 (88%)	391 (98%)	6 (2%)	0	100	100
1	H	397/453 (88%)	390 (98%)	7 (2%)	0	100	100
All	All	3176/3624 (88%)	3119 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/351 (88%)	286 (93%)	21 (7%)	16	25
1	B	307/351 (88%)	285 (93%)	22 (7%)	14	23
1	C	307/351 (88%)	285 (93%)	22 (7%)	14	23
1	D	307/351 (88%)	285 (93%)	22 (7%)	14	23
1	E	307/351 (88%)	285 (93%)	22 (7%)	14	23
1	F	307/351 (88%)	286 (93%)	21 (7%)	16	25
1	G	307/351 (88%)	285 (93%)	22 (7%)	14	23
1	H	307/351 (88%)	284 (92%)	23 (8%)	13	21
All	All	2456/2808 (88%)	2281 (93%)	175 (7%)	14	23

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ARG
1	A	29	GLU
1	A	57	LEU
1	A	96	TYR
1	A	106	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	139	LEU
1	A	161	PHE
1	A	166	LYS
1	A	170	LEU
1	A	171	LEU
1	A	184	GLN
1	A	218	THR
1	A	237	PHE
1	A	256	LEU
1	A	274	ARG
1	A	282	ARG
1	A	309	LEU
1	A	338	ARG
1	A	344	LYS
1	A	363	VAL
1	A	412	ILE
1	B	25	ARG
1	B	29	GLU
1	B	57	LEU
1	B	96	TYR
1	B	106	LEU
1	B	139	LEU
1	B	161	PHE
1	B	166	LYS
1	B	170	LEU
1	B	171	LEU
1	B	173	VAL
1	B	184	GLN
1	B	218	THR
1	B	237	PHE
1	B	256	LEU
1	B	274	ARG
1	B	282	ARG
1	B	309	LEU
1	B	338	ARG
1	B	344	LYS
1	B	363	VAL
1	B	412	ILE
1	C	25	ARG
1	C	29	GLU
1	C	57	LEU
1	C	96	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	106	LEU
1	C	139	LEU
1	C	161	PHE
1	C	166	LYS
1	C	170	LEU
1	C	171	LEU
1	C	173	VAL
1	C	184	GLN
1	C	218	THR
1	C	237	PHE
1	C	256	LEU
1	C	274	ARG
1	C	282	ARG
1	C	309	LEU
1	C	338	ARG
1	C	344	LYS
1	C	363	VAL
1	C	412	ILE
1	D	25	ARG
1	D	29	GLU
1	D	57	LEU
1	D	96	TYR
1	D	106	LEU
1	D	139	LEU
1	D	161	PHE
1	D	166	LYS
1	D	170	LEU
1	D	171	LEU
1	D	173	VAL
1	D	184	GLN
1	D	218	THR
1	D	237	PHE
1	D	256	LEU
1	D	274	ARG
1	D	282	ARG
1	D	309	LEU
1	D	338	ARG
1	D	344	LYS
1	D	363	VAL
1	D	412	ILE
1	E	25	ARG
1	E	29	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	57	LEU
1	E	96	TYR
1	E	106	LEU
1	E	139	LEU
1	E	161	PHE
1	E	166	LYS
1	E	170	LEU
1	E	171	LEU
1	E	173	VAL
1	E	184	GLN
1	E	218	THR
1	E	237	PHE
1	E	256	LEU
1	E	274	ARG
1	E	282	ARG
1	E	309	LEU
1	E	338	ARG
1	E	344	LYS
1	E	363	VAL
1	E	412	ILE
1	F	25	ARG
1	F	29	GLU
1	F	57	LEU
1	F	96	TYR
1	F	106	LEU
1	F	139	LEU
1	F	161	PHE
1	F	166	LYS
1	F	170	LEU
1	F	171	LEU
1	F	173	VAL
1	F	184	GLN
1	F	218	THR
1	F	237	PHE
1	F	256	LEU
1	F	274	ARG
1	F	282	ARG
1	F	309	LEU
1	F	338	ARG
1	F	344	LYS
1	F	363	VAL
1	G	25	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	G	29	GLU
1	G	57	LEU
1	G	96	TYR
1	G	106	LEU
1	G	139	LEU
1	G	161	PHE
1	G	166	LYS
1	G	170	LEU
1	G	171	LEU
1	G	173	VAL
1	G	184	GLN
1	G	218	THR
1	G	237	PHE
1	G	256	LEU
1	G	274	ARG
1	G	282	ARG
1	G	309	LEU
1	G	338	ARG
1	G	344	LYS
1	G	363	VAL
1	G	412	ILE
1	H	25	ARG
1	H	29	GLU
1	H	34	THR
1	H	57	LEU
1	H	96	TYR
1	H	106	LEU
1	H	139	LEU
1	H	161	PHE
1	H	166	LYS
1	H	170	LEU
1	H	171	LEU
1	H	173	VAL
1	H	184	GLN
1	H	218	THR
1	H	237	PHE
1	H	256	LEU
1	H	274	ARG
1	H	282	ARG
1	H	309	LEU
1	H	338	ARG
1	H	344	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	363	VAL
1	H	412	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	HIS
1	E	100	ASN
1	H	221	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	399/453 (88%)	0.25	25 (6%) 20 18	25, 45, 73, 105	0
1	B	399/453 (88%)	0.31	30 (7%) 14 13	27, 48, 73, 104	0
1	C	399/453 (88%)	0.10	4 (1%) 82 80	26, 43, 69, 102	0
1	D	399/453 (88%)	0.18	17 (4%) 35 33	26, 46, 71, 103	0
1	E	399/453 (88%)	0.05	9 (2%) 60 58	25, 44, 70, 104	0
1	F	399/453 (88%)	0.35	28 (7%) 16 15	26, 48, 72, 103	0
1	G	399/453 (88%)	0.05	4 (1%) 82 80	26, 44, 70, 101	0
1	H	399/453 (88%)	0.14	17 (4%) 35 33	25, 46, 73, 102	0
All	All	3192/3624 (88%)	0.18	134 (4%) 36 35	25, 45, 71, 105	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	HIS	8.9
1	F	221	HIS	7.8
1	A	180	ASP	6.1
1	A	138	VAL	6.1
1	A	139	LEU	5.8
1	B	221	HIS	5.8
1	A	242	ILE	5.6
1	E	180	ASP	5.4
1	A	140	ASP	5.0
1	A	243	GLN	4.9
1	B	149	GLU	4.6
1	A	132	SER	4.5
1	A	184	GLN	4.4
1	H	145	ALA	4.3
1	A	181	SER	4.3
1	F	154	VAL	4.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	147	PRO	4.3
1	E	181	SER	4.2
1	F	148	THR	4.2
1	D	239	LEU	4.2
1	B	179	ASP	4.1
1	D	161	PHE	4.1
1	D	111	GLU	4.0
1	F	149	GLU	3.8
1	B	152	GLY	3.8
1	B	332	ALA	3.8
1	A	185	GLY	3.7
1	F	65	GLU	3.7
1	A	237	PHE	3.6
1	F	180	ASP	3.6
1	G	32	ARG	3.6
1	F	120	ILE	3.4
1	D	139	LEU	3.4
1	B	117	TYR	3.4
1	B	148	THR	3.3
1	B	180	ASP	3.3
1	B	66	TYR	3.3
1	B	146	THR	3.3
1	F	111	GLU	3.3
1	B	233	ALA	3.3
1	H	178	GLN	3.3
1	H	139	LEU	3.2
1	D	149	GLU	3.2
1	B	190	ALA	3.2
1	B	65	GLU	3.2
1	B	123	ASN	3.1
1	B	197	ALA	3.1
1	B	104	ILE	3.1
1	H	66	TYR	3.1
1	D	244	SER	3.1
1	H	111	GLU	3.0
1	A	149	GLU	3.0
1	B	161	PHE	3.0
1	D	180	ASP	3.0
1	H	161	PHE	3.0
1	F	104	ILE	2.8
1	A	187	ILE	2.8
1	B	110	GLN	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	188	ILE	2.7
1	F	183	GLN	2.7
1	B	227	PRO	2.7
1	G	149	GLU	2.7
1	A	178	GLN	2.7
1	A	67	GLY	2.7
1	E	182	PRO	2.7
1	C	149	GLU	2.7
1	A	183	GLN	2.7
1	F	153	TYR	2.7
1	F	150	ASP	2.6
1	E	161	PHE	2.6
1	F	224	LYS	2.6
1	F	66	TYR	2.6
1	D	243	GLN	2.6
1	H	185	GLY	2.6
1	F	227	PRO	2.6
1	F	161	PHE	2.6
1	B	111	GLU	2.6
1	D	109	SER	2.6
1	A	182	PRO	2.6
1	F	63	PRO	2.5
1	B	63	PRO	2.5
1	F	116	LEU	2.5
1	B	114	GLU	2.5
1	A	176	VAL	2.5
1	D	185	GLY	2.5
1	F	291	GLN	2.4
1	H	149	GLU	2.4
1	F	119	GLN	2.4
1	D	158	THR	2.4
1	H	122	GLN	2.4
1	H	238	VAL	2.4
1	F	147	PRO	2.4
1	E	242	ILE	2.3
1	F	123	ASN	2.3
1	D	332	ALA	2.3
1	A	151	GLY	2.3
1	B	116	LEU	2.3
1	H	110	GLN	2.3
1	C	40	ARG	2.2
1	H	151	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	228	ASP	2.2
1	H	228	ASP	2.2
1	H	109	SER	2.2
1	B	232	GLY	2.2
1	C	32	ARG	2.2
1	F	230	VAL	2.2
1	A	179	ASP	2.2
1	D	235	ASN	2.2
1	A	145	ALA	2.2
1	D	32	ARG	2.1
1	D	151	GLY	2.1
1	B	150	ASP	2.1
1	E	64	ARG	2.1
1	E	149	GLU	2.1
1	A	154	VAL	2.1
1	B	291	GLN	2.1
1	D	182	PRO	2.1
1	F	55	SER	2.1
1	B	151	GLY	2.1
1	F	182	PRO	2.1
1	G	139	LEU	2.1
1	G	161	PHE	2.1
1	H	119	GLN	2.1
1	E	221	HIS	2.1
1	F	188	ILE	2.0
1	B	231	LEU	2.0
1	A	142	LYS	2.0
1	C	35	ALA	2.0
1	E	237	PHE	2.0
1	F	67	GLY	2.0
1	H	152	GLY	2.0
1	D	237	PHE	2.0
1	H	96	TYR	2.0
1	B	228	ASP	2.0

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

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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.