



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:22 PM UTC

PDB ID : 4JEK / pdb_00004jek
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

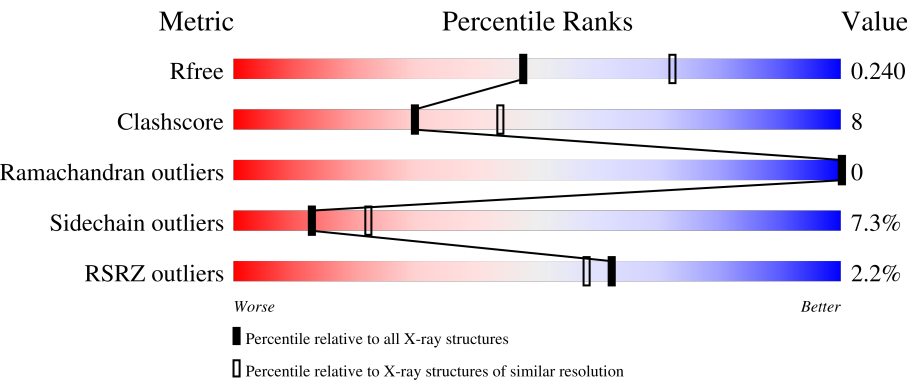
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	6% 67%18%•12%
1	B	453	2% 67%18%•12%
1	C	453	% 69%17%•12%
1	D	453	2% 68%18%•12%
1	E	453	% 72%13%•12%

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Mol	Chain	Length	Quality of chain
1	F	453	% 69% 17% • 12%
1	G	453	% 69% 17% • 12%
1	H	453	% 68% 18% • 12%

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

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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

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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

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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

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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

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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

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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

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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

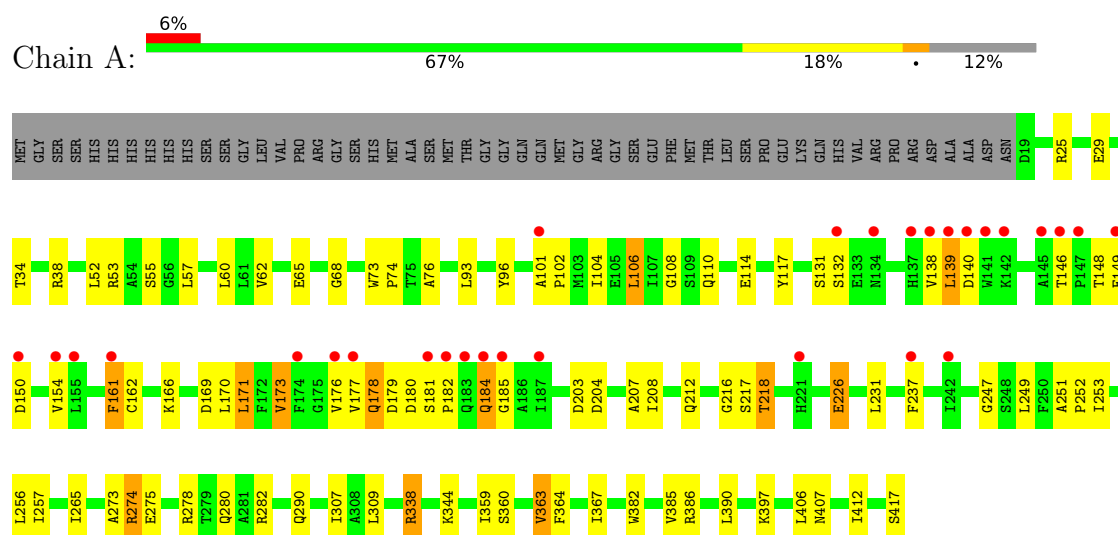
- Molecule 2 is water.

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

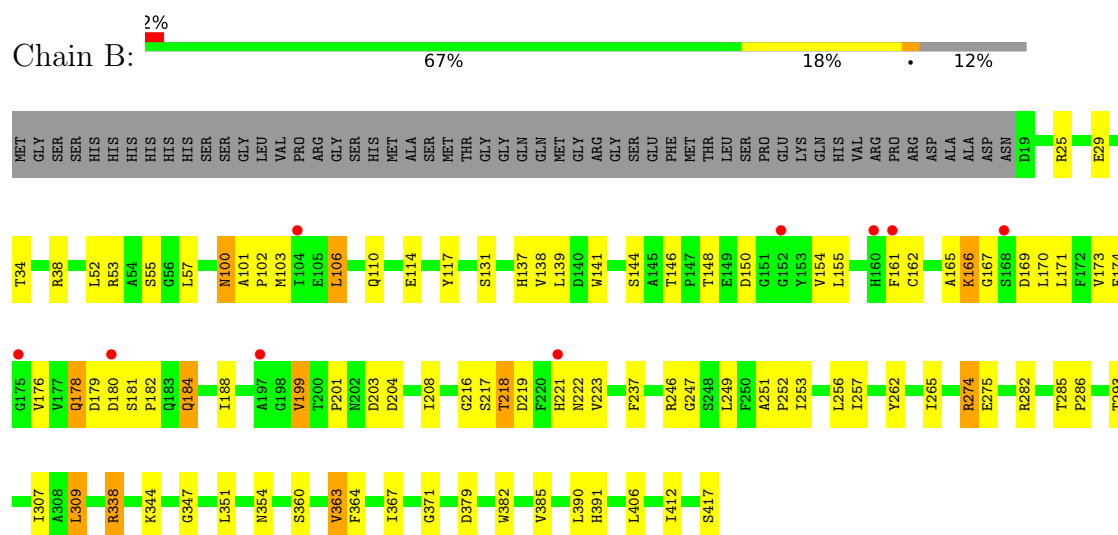
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

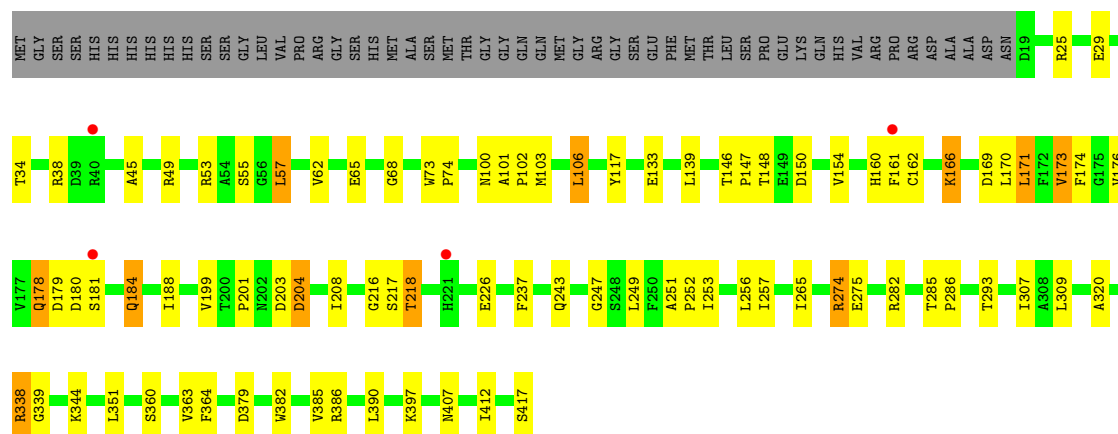


• Molecule 1: Dibenzothiophene desulfurization enzyme C

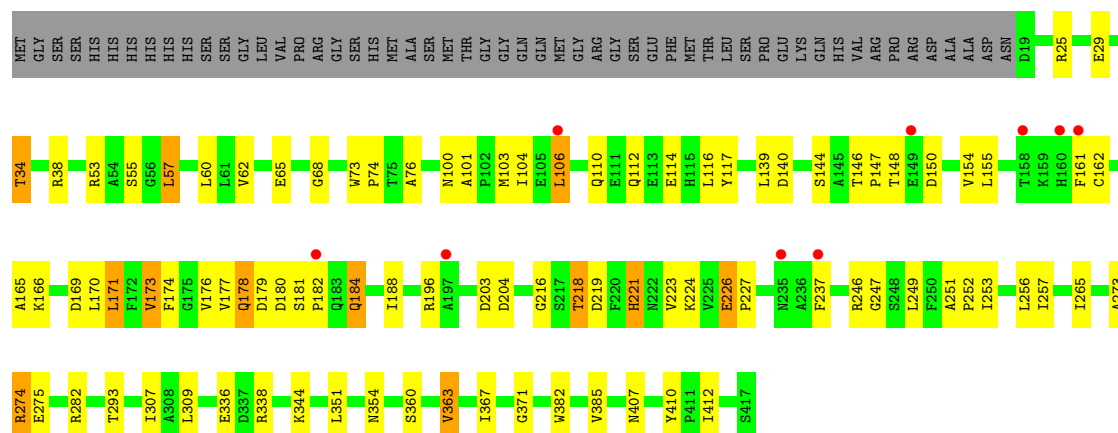


• Molecule 1: Dibenzothiophene desulfurization enzyme C

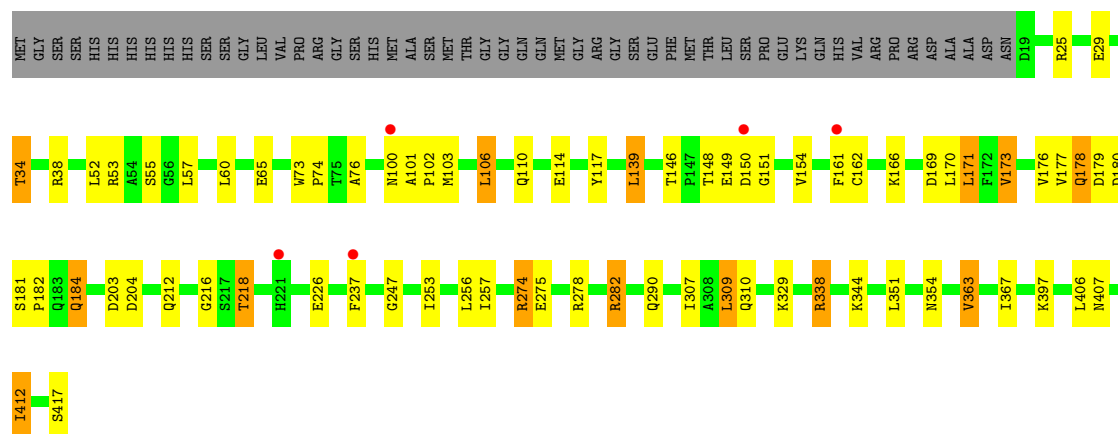
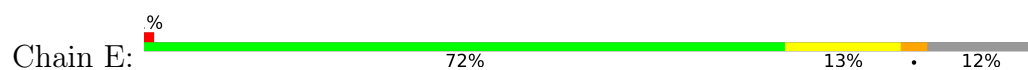




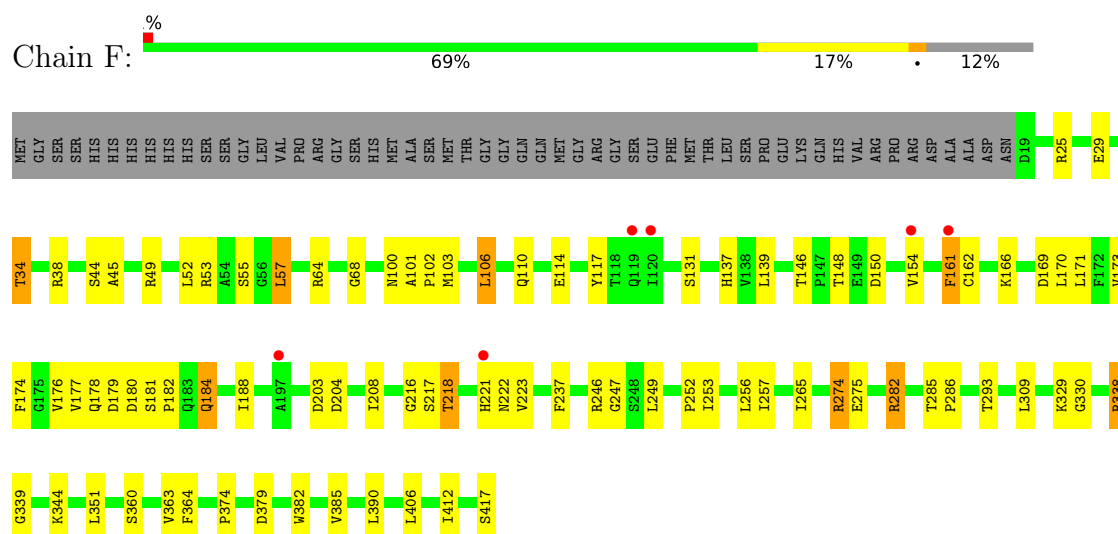
• Molecule 1: Dibenzothiophene desulfurization enzyme C



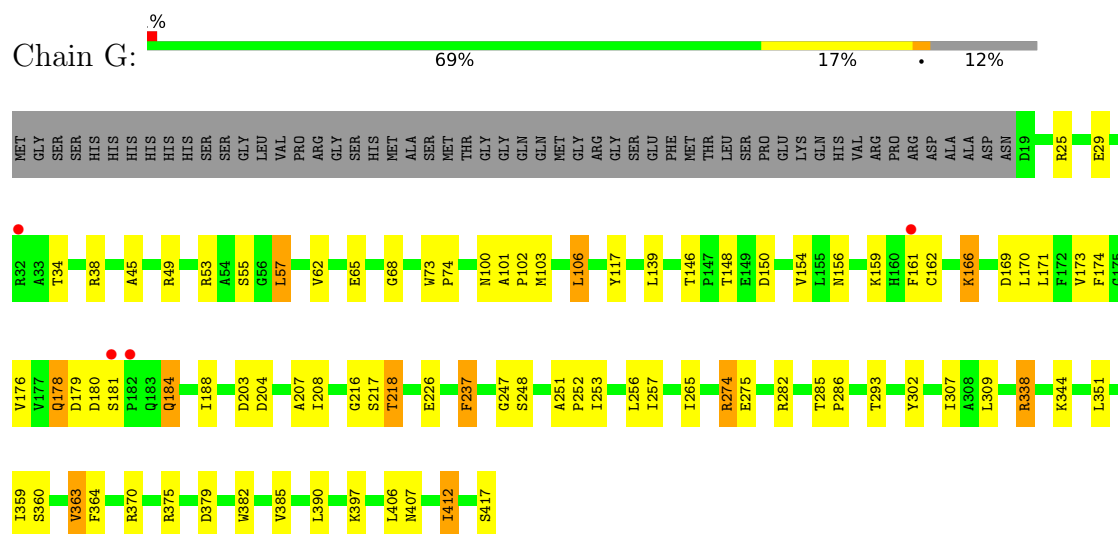
• Molecule 1: Dibenzothiophene desulfurization enzyme C



• Molecule 1: Dibenzothiophene desulfurization enzyme C



- 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, α , β , γ	96.16Å 96.27Å 98.56Å 81.03° 67.57° 85.84°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.2 (40.00-2.40) 96.7 (40.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.207 , 0.246 0.205 , 0.240	Depositor DCC
R_{free} test set	3843 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.530	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	24898	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.83	0/3116	0.95	3/4248 (0.1%)
1	B	0.83	2/3116 (0.1%)	0.94	1/4248 (0.0%)
1	C	0.82	1/3116 (0.0%)	0.95	4/4248 (0.1%)
1	D	0.82	1/3116 (0.0%)	0.94	2/4248 (0.0%)
1	E	0.82	0/3116	0.95	1/4248 (0.0%)
1	F	0.81	0/3116	0.92	0/4248
1	G	0.81	0/3116	0.93	2/4248 (0.0%)
1	H	0.79	0/3116	0.91	0/4248
All	All	0.82	4/24928 (0.0%)	0.94	13/33984 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	100	ASN	CG-ND2	-8.04	1.16	1.33
1	B	100	ASN	CG-OD1	-7.29	1.09	1.23
1	C	160	HIS	CE1-NE2	-6.15	1.26	1.32
1	D	221	HIS	CE1-NE2	-5.59	1.26	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LYS	N-CA-C	-5.86	104.81	111.14
1	C	204	ASP	N-CA-CB	-5.57	103.49	110.90
1	E	397	LYS	N-CA-C	-5.55	105.31	111.36
1	G	397	LYS	N-CA-C	-5.51	105.35	111.36
1	A	226	GLU	CA-C-N	5.50	125.59	119.32
1	A	226	GLU	C-N-CA	5.50	125.59	119.32
1	D	226	GLU	CA-C-N	5.35	125.41	119.32
1	D	226	GLU	C-N-CA	5.35	125.41	119.32
1	C	386	ARG	N-CA-C	-5.32	105.64	111.82
1	C	166	LYS	N-CA-C	5.28	117.46	111.02
1	C	397	LYS	N-CA-C	-5.23	105.66	111.36
1	B	199	VAL	CB-CA-C	-5.13	105.69	111.23
1	G	166	LYS	N-CA-C	5.01	117.13	111.11

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	67	7
1	B	3041	0	2918	64	2
1	C	3041	0	2918	45	5
1	D	3041	0	2918	62	0
1	E	3041	0	2918	42	3
1	F	3041	0	2918	54	2
1	G	3041	0	2918	49	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	403	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 (403) 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

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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

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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: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:F:148:THR:OG1	1:F:150:ASP:OD1	2.18	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:204:ASP:OD2	1:B:217:SER:OG	2.18	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:B:137:HIS:CB	1:H:221:HIS:NE2	2.67	0.57
1:D:196:ARG:HD2	2:D:557:HOH:O	2.03	0.57
1:F:339:GLY:HA2	2:F:512:HOH:O	2.04	0.57
1:G:204:ASP:OD2	1:G:217:SER:OG	2.11	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:A:148:THR:OG1	1:A:150:ASP:OD1	2.19	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:B:347:GLY:HA3	1:E:310:GLN:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:THR:HB	1:E:154:VAL:HG23	1.88	0.56
1:H:162:CYS:SG	1:H:218:THR:HG23	2.46	0.56
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:148:THR:OG1	1:E:150:ASP:OD1	2.18	0.54
1:F:204:ASP:OD2	1:F:217:SER:OG	2.17	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:F:52:LEU:O	1:F:55:SER:OG	2.23	0.53
1:A:274:ARG:HG3	1:A:275:GLU:N	2.24	0.53
1:C:148:THR:OG1	1:C:150:ASP:OD1	2.22	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:G:148:THR:OG1	1:G:150:ASP:OD1	2.19	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:H:34:THR:OG1	1:H:38:ARG:NH1	2.42	0.52
1:H:249:LEU:C	1:H:252:PRO:HD2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:52:LEU:O	1:B:55:SER:OG	2.24	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
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: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:D:249:LEU:C	1:D:252:PRO:HD2	2.37	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:A:204:ASP:OD2	1:A:217:SER:OG	2.15	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:A:407:ASN:OD1	1:F:293:THR:HB	2.12	0.48
1:B:146:THR:HB	1:B:154:VAL:HG23	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:360:SER:HB3	1:H:382:TRP:HB2	1.95	0.48
1:B:293:THR:HA	1:E:406:LEU:HD21	1.95	0.48
1:C:293:THR:HB	1:D:407:ASN:OD1	2.14	0.48
1:A:406:LEU:HD21	1:F:293:THR:HA	1.96	0.48
1:E:101:ALA:HB1	1:E:117:TYR:HE1	1.79	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
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:H:148:THR:OG1	1:H:150:ASP:OD1	2.22	0.47
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:B:179:ASP:O	1:B:180:ASP:HB2	2.13	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: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:H:251:ALA:N	1:H:252:PRO:CD	2.78	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:F:249:LEU:C	1:F:252:PRO:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:HG3	1:C:275:GLU:N	2.31	0.46
1:G:62:VAL:O	1:G:68:GLY:HA3	2.16	0.46
1:G:179:ASP:O	1:G:180:ASP:HB2	2.15	0.46
1:A:307:ILE:HG23	1:F:351:LEU:HG	1.97	0.46
1:C:179:ASP:HB3	1:C:181:SER:H	1.80	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:363:VAL:HG13	1:B:367:ILE:HD12	1.97	0.46
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: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:HD12	1:A:139:LEU:HA	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: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:73:TRP:HB2	1:D:74:PRO:HD3	1.99	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: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:45:ALA:O	1:H:49:ARG:HG3	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:E:309:LEU:HA	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
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: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:F:100:ASN:O	1:F:103:MET:HB3	2.18	0.44
1:A:38:ARG:HB3	1:A:212:GLN:OE1	2.18	0.44
1:A:101:ALA:HB1	1:A:117:TYR:HE1	1.83	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:60:LEU:HD21	1:A:76:ALA:HA	2.00	0.43
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: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:249:LEU:C	1:A:252:PRO:HD2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:52:LEU:O	1:E:55:SER:OG	2.31	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: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:62:VAL:O	1:C:68:GLY:HA3	2.20	0.41
1:C:204:ASP:OD2	1:C:217:SER:OG	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HG	1:D:307:ILE:HG23	2.02	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:249:LEU:C	1:B:252:PRO:HD2	2.46	0.41
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.78	0.41
1:F:329:LYS:O	1:F:330:GLY:C	2.60	0.41
1:A:360:SER:HB3	1:A:382:TRP:HB2	2.02	0.41
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:N	1:B:262:TYR:CD1	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: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: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: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:G:412:ILE:H	1:G:412:ILE:HG12	1.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:LEU:HD12	1:E:139:LEU:HA	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
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:C:249:LEU:C	1:C:252:PRO:HD2	2.46	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 ⓘ

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	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
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%)	284 (92%)	23 (8%)	12	21
1	B	307/351 (88%)	286 (93%)	21 (7%)	14	25
1	C	307/351 (88%)	285 (93%)	22 (7%)	13	23
1	D	307/351 (88%)	284 (92%)	23 (8%)	12	21
1	E	307/351 (88%)	284 (92%)	23 (8%)	12	21
1	F	307/351 (88%)	285 (93%)	22 (7%)	13	23
1	G	307/351 (88%)	285 (93%)	22 (7%)	13	23
1	H	307/351 (88%)	284 (92%)	23 (8%)	12	21
All	All	2456/2808 (88%)	2277 (93%)	179 (7%)	13	22

All (179) 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	65	GLU
1	A	96	TYR
1	A	106	LEU
1	A	139	LEU
1	A	161	PHE
1	A	166	LYS
1	A	170	LEU
1	A	171	LEU
1	A	173	VAL
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	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

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Mol	Chain	Res	Type
1	B	412	ILE
1	C	25	ARG
1	C	29	GLU
1	C	57	LEU
1	C	65	GLU
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	34	THR
1	D	57	LEU
1	D	65	GLU
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

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Mol	Chain	Res	Type
1	D	338	ARG
1	D	344	LYS
1	D	363	VAL
1	D	412	ILE
1	E	25	ARG
1	E	29	GLU
1	E	34	THR
1	E	57	LEU
1	E	65	GLU
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	34	THR
1	F	57	LEU
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

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Mol	Chain	Res	Type
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	F	412	ILE
1	G	25	ARG
1	G	29	GLU
1	G	57	LEU
1	G	65	GLU
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	65	GLU
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

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

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

Mol	Chain	Res	Type
1	B	100	ASN
1	B	137	HIS
1	E	100	ASN
1	F	137	HIS
1	G	221	HIS
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 oligosaccharides 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, 95th 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(Å²)	Q<0.9
1	A	399/453 (88%)	0.29	29 (7%)	21	17	25, 45, 73, 105	0
1	B	399/453 (88%)	0.28	9 (2%)	61	57	27, 48, 73, 104	0
1	C	399/453 (88%)	0.09	4 (1%)	79	76	26, 43, 69, 102	0
1	D	399/453 (88%)	0.13	9 (2%)	61	57	26, 46, 71, 103	0
1	E	399/453 (88%)	0.02	5 (1%)	75	71	25, 44, 70, 104	0
1	F	399/453 (88%)	0.21	6 (1%)	72	68	26, 48, 72, 103	0
1	G	399/453 (88%)	0.10	4 (1%)	79	76	26, 44, 70, 101	0
1	H	399/453 (88%)	0.05	5 (1%)	75	71	25, 46, 73, 102	0
All	All	3192/3624 (88%)	0.15	71 (2%)	62	58	25, 45, 71, 105	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	161	PHE	4.9
1	A	138	VAL	4.9
1	F	221	HIS	4.9
1	A	140	ASP	4.6
1	A	137	HIS	4.4
1	H	161	PHE	4.1
1	B	221	HIS	4.1
1	A	132	SER	4.0
1	E	161	PHE	3.9
1	B	161	PHE	3.8
1	A	237	PHE	3.7
1	G	161	PHE	3.6
1	A	177	VAL	3.4
1	A	161	PHE	3.3
1	C	161	PHE	3.3
1	A	154	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	182	PRO	3.2
1	A	145	ALA	3.2
1	A	242	ILE	3.2
1	A	187	ILE	3.0
1	A	147	PRO	2.9
1	A	150	ASP	2.9
1	A	185	GLY	2.9
1	A	142	LYS	2.8
1	A	184	GLN	2.8
1	E	221	HIS	2.8
1	H	291	GLN	2.7
1	H	145	ALA	2.7
1	A	139	LEU	2.7
1	F	161	PHE	2.7
1	A	149	GLU	2.6
1	A	176	VAL	2.6
1	F	120	ILE	2.5
1	E	237	PHE	2.5
1	F	154	VAL	2.5
1	C	221	HIS	2.5
1	A	221	HIS	2.5
1	A	174	PHE	2.4
1	B	197	ALA	2.4
1	D	235	ASN	2.4
1	G	181	SER	2.4
1	G	182	PRO	2.3
1	A	183	GLN	2.3
1	B	104	ILE	2.3
1	A	146	THR	2.3
1	A	141	TRP	2.3
1	D	149	GLU	2.3
1	G	32	ARG	2.3
1	E	150	ASP	2.3
1	A	181	SER	2.2
1	D	237	PHE	2.2
1	D	182	PRO	2.2
1	D	106	LEU	2.2
1	D	158	THR	2.2
1	A	134	ASN	2.1
1	H	182	PRO	2.1
1	B	160	HIS	2.1
1	B	175	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	197	ALA	2.1
1	C	40	ARG	2.1
1	B	180	ASP	2.1
1	D	197	ALA	2.0
1	B	152	GLY	2.0
1	D	160	HIS	2.0
1	H	160	HIS	2.0
1	F	119	GLN	2.0
1	A	101	ALA	2.0
1	A	155	LEU	2.0
1	E	100	ASN	2.0
1	B	168	SER	2.0
1	C	181	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.