Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 09:18 PM EST

PDB ID	:	5ING
Title	:	A crotonyl-CoA reductase-carboxylase independent pathway for assembly of unusual alkylmalonyl-CoA polyketide synthase extender unit
Authors	:	Valentic, T.R.; Ray, L.; Miyazawa, T.; Song, L.; Withall, D.M.; Milligan, J.C.; Takahashi, S.; Osada, H.; Tsai, S.C.; Challis, G.L.
Deposited on	:	2016-03-07
Resolution	:	2.45 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 (i) 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 (i)) were used in the production of this report:

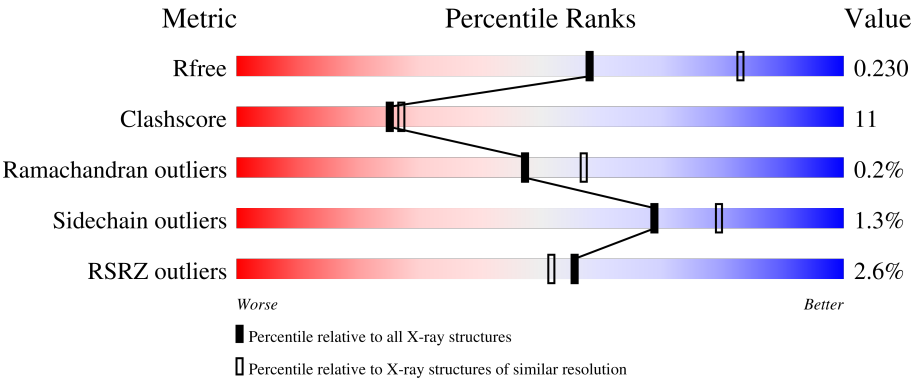
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 <=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	570	% 71% 16% • 13%
1	B	570	2% 72% 15% • 13%
1	C	570	3% 70% 16% • 12%
1	D	570	2% 70% 15% 14%
1	E	570	4% 68% 18% • 14%

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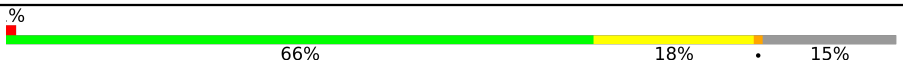
Mol	Chain	Length	Quality of chain
1	F	570	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 23360 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 Putative carboxyl transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	0	0	0
			3760	2366	661	714	6	13			
1	B	497	Total	C	N	O	S	Se	0	0	0
			3763	2368	662	714	6	13			
1	C	503	Total	C	N	O	S	Se	0	0	0
			3806	2394	670	723	6	13			
1	D	488	Total	C	N	O	S	Se	0	0	0
			3700	2329	653	699	6	13			
1	E	493	Total	C	N	O	S	Se	0	0	0
			3735	2349	659	709	6	12			
1	F	483	Total	C	N	O	S	Se	0	0	0
			3660	2303	648	690	6	13			

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-37	MSE	-	initiating methionine	UNP A0ACI9
A	-36	GLY	-	expression tag	UNP A0ACI9
A	-35	SER	-	expression tag	UNP A0ACI9
A	-34	SER	-	expression tag	UNP A0ACI9
A	-33	HIS	-	expression tag	UNP A0ACI9
A	-32	HIS	-	expression tag	UNP A0ACI9
A	-31	HIS	-	expression tag	UNP A0ACI9
A	-30	HIS	-	expression tag	UNP A0ACI9
A	-29	HIS	-	expression tag	UNP A0ACI9
A	-28	HIS	-	expression tag	UNP A0ACI9
A	-27	SER	-	expression tag	UNP A0ACI9
A	-26	SER	-	expression tag	UNP A0ACI9
A	-25	GLY	-	expression tag	UNP A0ACI9
A	-24	LEU	-	expression tag	UNP A0ACI9
A	-23	VAL	-	expression tag	UNP A0ACI9
A	-22	PRO	-	expression tag	UNP A0ACI9
A	-21	ARG	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	expression tag	UNP A0ACI9
A	-19	SER	-	expression tag	UNP A0ACI9
A	-18	HIS	-	expression tag	UNP A0ACI9
A	-17	MSE	-	expression tag	UNP A0ACI9
A	-16	ALA	-	expression tag	UNP A0ACI9
A	-15	SER	-	expression tag	UNP A0ACI9
A	-14	ASP	-	expression tag	UNP A0ACI9
A	-13	SER	-	expression tag	UNP A0ACI9
A	-12	THR	-	expression tag	UNP A0ACI9
A	-11	GLU	-	expression tag	UNP A0ACI9
A	-10	ASN	-	expression tag	UNP A0ACI9
A	-9	LEU	-	expression tag	UNP A0ACI9
A	-8	TYR	-	expression tag	UNP A0ACI9
A	-7	PHE	-	expression tag	UNP A0ACI9
A	-6	GLN	-	expression tag	UNP A0ACI9
A	-5	GLY	-	expression tag	UNP A0ACI9
A	-4	ILE	-	expression tag	UNP A0ACI9
A	-3	ASP	-	expression tag	UNP A0ACI9
A	-2	PRO	-	expression tag	UNP A0ACI9
A	-1	PHE	-	expression tag	UNP A0ACI9
A	0	THR	-	expression tag	UNP A0ACI9
A	1	MSE	-	expression tag	UNP A0ACI9
B	-37	MSE	-	initiating methionine	UNP A0ACI9
B	-36	GLY	-	expression tag	UNP A0ACI9
B	-35	SER	-	expression tag	UNP A0ACI9
B	-34	SER	-	expression tag	UNP A0ACI9
B	-33	HIS	-	expression tag	UNP A0ACI9
B	-32	HIS	-	expression tag	UNP A0ACI9
B	-31	HIS	-	expression tag	UNP A0ACI9
B	-30	HIS	-	expression tag	UNP A0ACI9
B	-29	HIS	-	expression tag	UNP A0ACI9
B	-28	HIS	-	expression tag	UNP A0ACI9
B	-27	SER	-	expression tag	UNP A0ACI9
B	-26	SER	-	expression tag	UNP A0ACI9
B	-25	GLY	-	expression tag	UNP A0ACI9
B	-24	LEU	-	expression tag	UNP A0ACI9
B	-23	VAL	-	expression tag	UNP A0ACI9
B	-22	PRO	-	expression tag	UNP A0ACI9
B	-21	ARG	-	expression tag	UNP A0ACI9
B	-20	GLY	-	expression tag	UNP A0ACI9
B	-19	SER	-	expression tag	UNP A0ACI9
B	-18	HIS	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MSE	-	expression tag	UNP A0ACI9
B	-16	ALA	-	expression tag	UNP A0ACI9
B	-15	SER	-	expression tag	UNP A0ACI9
B	-14	ASP	-	expression tag	UNP A0ACI9
B	-13	SER	-	expression tag	UNP A0ACI9
B	-12	THR	-	expression tag	UNP A0ACI9
B	-11	GLU	-	expression tag	UNP A0ACI9
B	-10	ASN	-	expression tag	UNP A0ACI9
B	-9	LEU	-	expression tag	UNP A0ACI9
B	-8	TYR	-	expression tag	UNP A0ACI9
B	-7	PHE	-	expression tag	UNP A0ACI9
B	-6	GLN	-	expression tag	UNP A0ACI9
B	-5	GLY	-	expression tag	UNP A0ACI9
B	-4	ILE	-	expression tag	UNP A0ACI9
B	-3	ASP	-	expression tag	UNP A0ACI9
B	-2	PRO	-	expression tag	UNP A0ACI9
B	-1	PHE	-	expression tag	UNP A0ACI9
B	0	THR	-	expression tag	UNP A0ACI9
B	1	MSE	-	expression tag	UNP A0ACI9
C	-37	MSE	-	initiating methionine	UNP A0ACI9
C	-36	GLY	-	expression tag	UNP A0ACI9
C	-35	SER	-	expression tag	UNP A0ACI9
C	-34	SER	-	expression tag	UNP A0ACI9
C	-33	HIS	-	expression tag	UNP A0ACI9
C	-32	HIS	-	expression tag	UNP A0ACI9
C	-31	HIS	-	expression tag	UNP A0ACI9
C	-30	HIS	-	expression tag	UNP A0ACI9
C	-29	HIS	-	expression tag	UNP A0ACI9
C	-28	HIS	-	expression tag	UNP A0ACI9
C	-27	SER	-	expression tag	UNP A0ACI9
C	-26	SER	-	expression tag	UNP A0ACI9
C	-25	GLY	-	expression tag	UNP A0ACI9
C	-24	LEU	-	expression tag	UNP A0ACI9
C	-23	VAL	-	expression tag	UNP A0ACI9
C	-22	PRO	-	expression tag	UNP A0ACI9
C	-21	ARG	-	expression tag	UNP A0ACI9
C	-20	GLY	-	expression tag	UNP A0ACI9
C	-19	SER	-	expression tag	UNP A0ACI9
C	-18	HIS	-	expression tag	UNP A0ACI9
C	-17	MSE	-	expression tag	UNP A0ACI9
C	-16	ALA	-	expression tag	UNP A0ACI9
C	-15	SER	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP A0ACI9
C	-13	SER	-	expression tag	UNP A0ACI9
C	-12	THR	-	expression tag	UNP A0ACI9
C	-11	GLU	-	expression tag	UNP A0ACI9
C	-10	ASN	-	expression tag	UNP A0ACI9
C	-9	LEU	-	expression tag	UNP A0ACI9
C	-8	TYR	-	expression tag	UNP A0ACI9
C	-7	PHE	-	expression tag	UNP A0ACI9
C	-6	GLN	-	expression tag	UNP A0ACI9
C	-5	GLY	-	expression tag	UNP A0ACI9
C	-4	ILE	-	expression tag	UNP A0ACI9
C	-3	ASP	-	expression tag	UNP A0ACI9
C	-2	PRO	-	expression tag	UNP A0ACI9
C	-1	PHE	-	expression tag	UNP A0ACI9
C	0	THR	-	expression tag	UNP A0ACI9
C	1	MSE	-	expression tag	UNP A0ACI9
D	-37	MSE	-	initiating methionine	UNP A0ACI9
D	-36	GLY	-	expression tag	UNP A0ACI9
D	-35	SER	-	expression tag	UNP A0ACI9
D	-34	SER	-	expression tag	UNP A0ACI9
D	-33	HIS	-	expression tag	UNP A0ACI9
D	-32	HIS	-	expression tag	UNP A0ACI9
D	-31	HIS	-	expression tag	UNP A0ACI9
D	-30	HIS	-	expression tag	UNP A0ACI9
D	-29	HIS	-	expression tag	UNP A0ACI9
D	-28	HIS	-	expression tag	UNP A0ACI9
D	-27	SER	-	expression tag	UNP A0ACI9
D	-26	SER	-	expression tag	UNP A0ACI9
D	-25	GLY	-	expression tag	UNP A0ACI9
D	-24	LEU	-	expression tag	UNP A0ACI9
D	-23	VAL	-	expression tag	UNP A0ACI9
D	-22	PRO	-	expression tag	UNP A0ACI9
D	-21	ARG	-	expression tag	UNP A0ACI9
D	-20	GLY	-	expression tag	UNP A0ACI9
D	-19	SER	-	expression tag	UNP A0ACI9
D	-18	HIS	-	expression tag	UNP A0ACI9
D	-17	MSE	-	expression tag	UNP A0ACI9
D	-16	ALA	-	expression tag	UNP A0ACI9
D	-15	SER	-	expression tag	UNP A0ACI9
D	-14	ASP	-	expression tag	UNP A0ACI9
D	-13	SER	-	expression tag	UNP A0ACI9
D	-12	THR	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	GLU	-	expression tag	UNP A0ACI9
D	-10	ASN	-	expression tag	UNP A0ACI9
D	-9	LEU	-	expression tag	UNP A0ACI9
D	-8	TYR	-	expression tag	UNP A0ACI9
D	-7	PHE	-	expression tag	UNP A0ACI9
D	-6	GLN	-	expression tag	UNP A0ACI9
D	-5	GLY	-	expression tag	UNP A0ACI9
D	-4	ILE	-	expression tag	UNP A0ACI9
D	-3	ASP	-	expression tag	UNP A0ACI9
D	-2	PRO	-	expression tag	UNP A0ACI9
D	-1	PHE	-	expression tag	UNP A0ACI9
D	0	THR	-	expression tag	UNP A0ACI9
D	1	MSE	-	expression tag	UNP A0ACI9
E	-37	MSE	-	initiating methionine	UNP A0ACI9
E	-36	GLY	-	expression tag	UNP A0ACI9
E	-35	SER	-	expression tag	UNP A0ACI9
E	-34	SER	-	expression tag	UNP A0ACI9
E	-33	HIS	-	expression tag	UNP A0ACI9
E	-32	HIS	-	expression tag	UNP A0ACI9
E	-31	HIS	-	expression tag	UNP A0ACI9
E	-30	HIS	-	expression tag	UNP A0ACI9
E	-29	HIS	-	expression tag	UNP A0ACI9
E	-28	HIS	-	expression tag	UNP A0ACI9
E	-27	SER	-	expression tag	UNP A0ACI9
E	-26	SER	-	expression tag	UNP A0ACI9
E	-25	GLY	-	expression tag	UNP A0ACI9
E	-24	LEU	-	expression tag	UNP A0ACI9
E	-23	VAL	-	expression tag	UNP A0ACI9
E	-22	PRO	-	expression tag	UNP A0ACI9
E	-21	ARG	-	expression tag	UNP A0ACI9
E	-20	GLY	-	expression tag	UNP A0ACI9
E	-19	SER	-	expression tag	UNP A0ACI9
E	-18	HIS	-	expression tag	UNP A0ACI9
E	-17	MSE	-	expression tag	UNP A0ACI9
E	-16	ALA	-	expression tag	UNP A0ACI9
E	-15	SER	-	expression tag	UNP A0ACI9
E	-14	ASP	-	expression tag	UNP A0ACI9
E	-13	SER	-	expression tag	UNP A0ACI9
E	-12	THR	-	expression tag	UNP A0ACI9
E	-11	GLU	-	expression tag	UNP A0ACI9
E	-10	ASN	-	expression tag	UNP A0ACI9
E	-9	LEU	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	TYR	-	expression tag	UNP A0ACI9
E	-7	PHE	-	expression tag	UNP A0ACI9
E	-6	GLN	-	expression tag	UNP A0ACI9
E	-5	GLY	-	expression tag	UNP A0ACI9
E	-4	ILE	-	expression tag	UNP A0ACI9
E	-3	ASP	-	expression tag	UNP A0ACI9
E	-2	PRO	-	expression tag	UNP A0ACI9
E	-1	PHE	-	expression tag	UNP A0ACI9
E	0	THR	-	expression tag	UNP A0ACI9
E	1	MSE	-	expression tag	UNP A0ACI9
F	-37	MSE	-	initiating methionine	UNP A0ACI9
F	-36	GLY	-	expression tag	UNP A0ACI9
F	-35	SER	-	expression tag	UNP A0ACI9
F	-34	SER	-	expression tag	UNP A0ACI9
F	-33	HIS	-	expression tag	UNP A0ACI9
F	-32	HIS	-	expression tag	UNP A0ACI9
F	-31	HIS	-	expression tag	UNP A0ACI9
F	-30	HIS	-	expression tag	UNP A0ACI9
F	-29	HIS	-	expression tag	UNP A0ACI9
F	-28	HIS	-	expression tag	UNP A0ACI9
F	-27	SER	-	expression tag	UNP A0ACI9
F	-26	SER	-	expression tag	UNP A0ACI9
F	-25	GLY	-	expression tag	UNP A0ACI9
F	-24	LEU	-	expression tag	UNP A0ACI9
F	-23	VAL	-	expression tag	UNP A0ACI9
F	-22	PRO	-	expression tag	UNP A0ACI9
F	-21	ARG	-	expression tag	UNP A0ACI9
F	-20	GLY	-	expression tag	UNP A0ACI9
F	-19	SER	-	expression tag	UNP A0ACI9
F	-18	HIS	-	expression tag	UNP A0ACI9
F	-17	MSE	-	expression tag	UNP A0ACI9
F	-16	ALA	-	expression tag	UNP A0ACI9
F	-15	SER	-	expression tag	UNP A0ACI9
F	-14	ASP	-	expression tag	UNP A0ACI9
F	-13	SER	-	expression tag	UNP A0ACI9
F	-12	THR	-	expression tag	UNP A0ACI9
F	-11	GLU	-	expression tag	UNP A0ACI9
F	-10	ASN	-	expression tag	UNP A0ACI9
F	-9	LEU	-	expression tag	UNP A0ACI9
F	-8	TYR	-	expression tag	UNP A0ACI9
F	-7	PHE	-	expression tag	UNP A0ACI9
F	-6	GLN	-	expression tag	UNP A0ACI9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-5	GLY	-	expression tag	UNP A0ACI9
F	-4	ILE	-	expression tag	UNP A0ACI9
F	-3	ASP	-	expression tag	UNP A0ACI9
F	-2	PRO	-	expression tag	UNP A0ACI9
F	-1	PHE	-	expression tag	UNP A0ACI9
F	0	THR	-	expression tag	UNP A0ACI9
F	1	MSE	-	expression tag	UNP A0ACI9

- Molecule 2 is water.

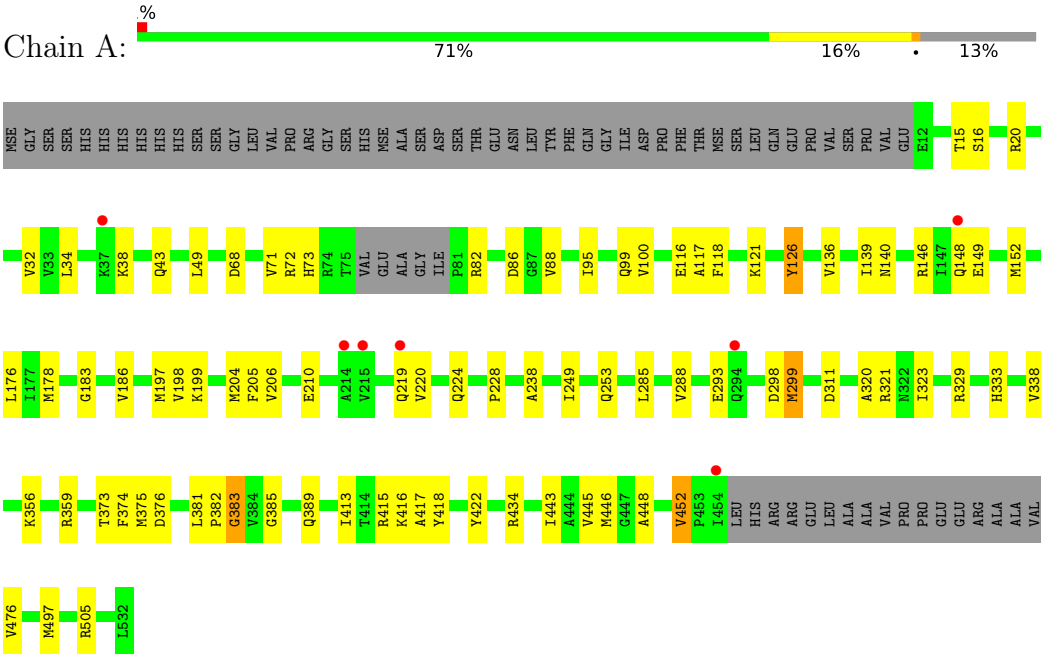
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	166	Total O 166 166	0	0
2	B	214	Total O 214 214	0	0
2	C	156	Total O 156 156	0	0
2	D	152	Total O 152 152	0	0
2	E	136	Total O 136 136	0	0
2	F	112	Total O 112 112	0	0

3 Residue-property plots (i)

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.

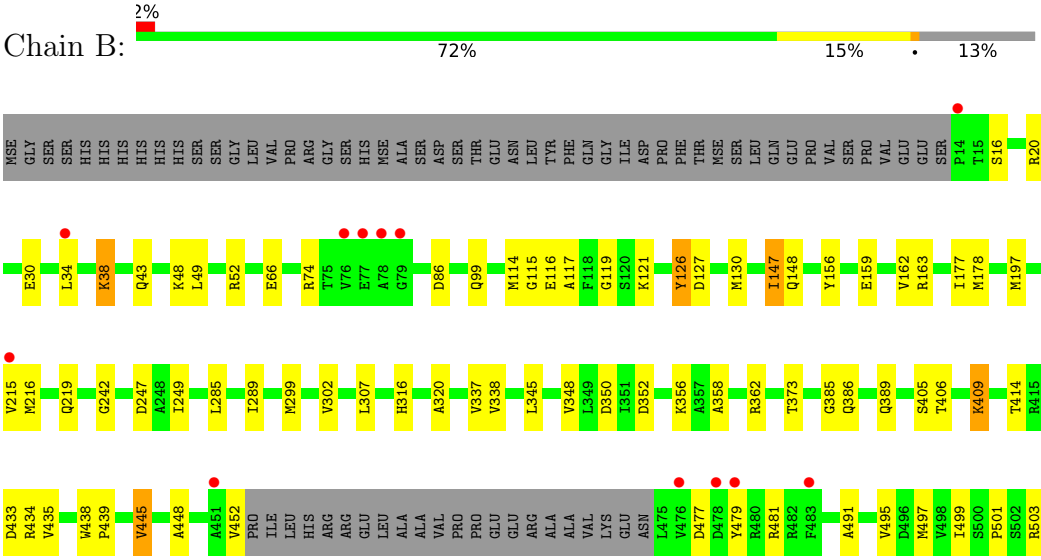
• Molecule 1: Putative carboxyl transferase

Chain A:

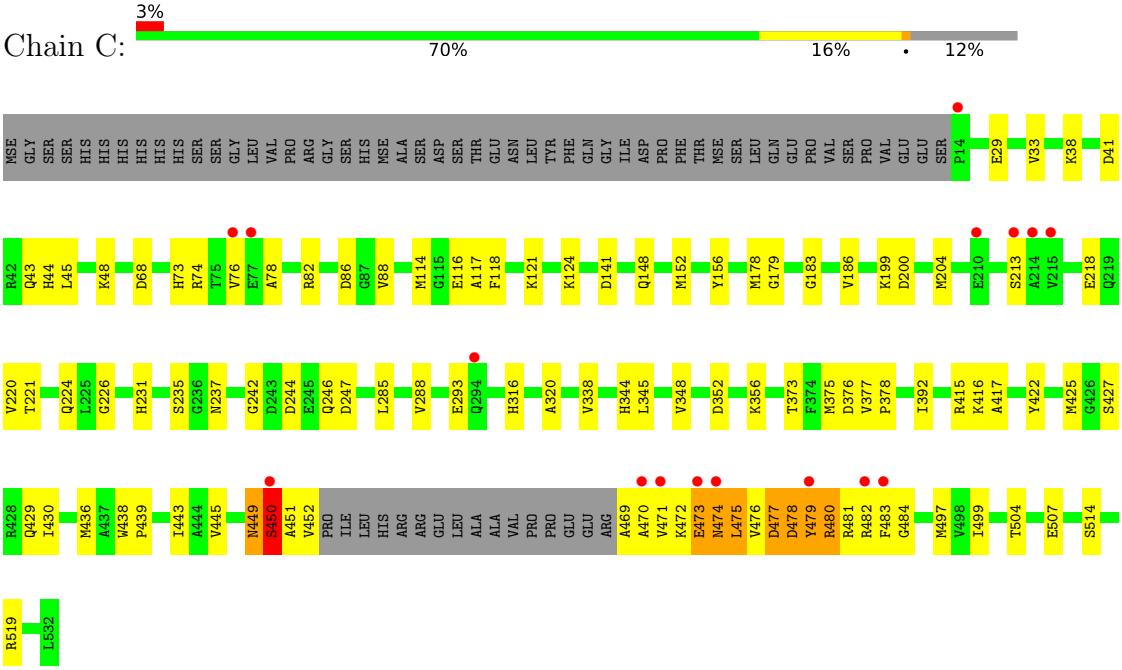


• Molecule 1: Putative carboxyl transferase

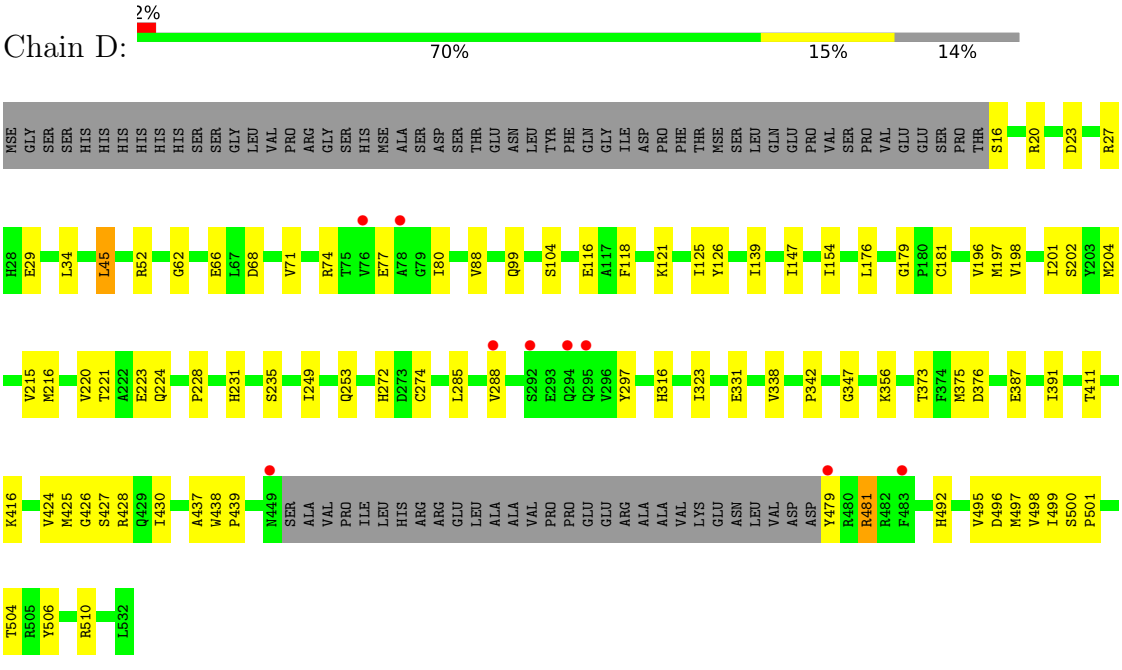
Chain B:



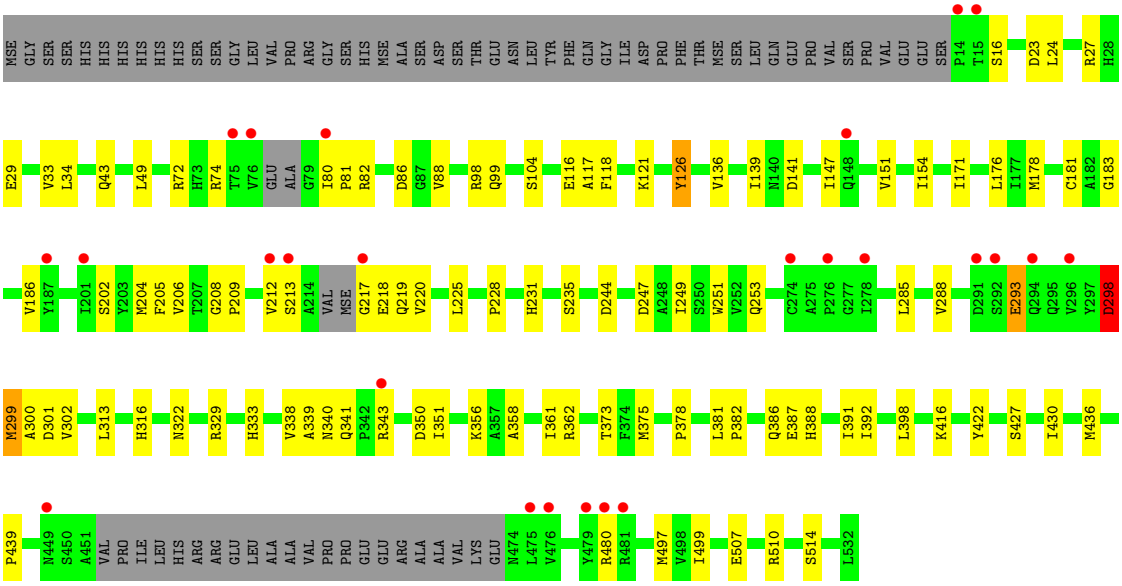
• Molecule 1: Putative carboxyl transferase



• Molecule 1: Putative carboxyl transferase

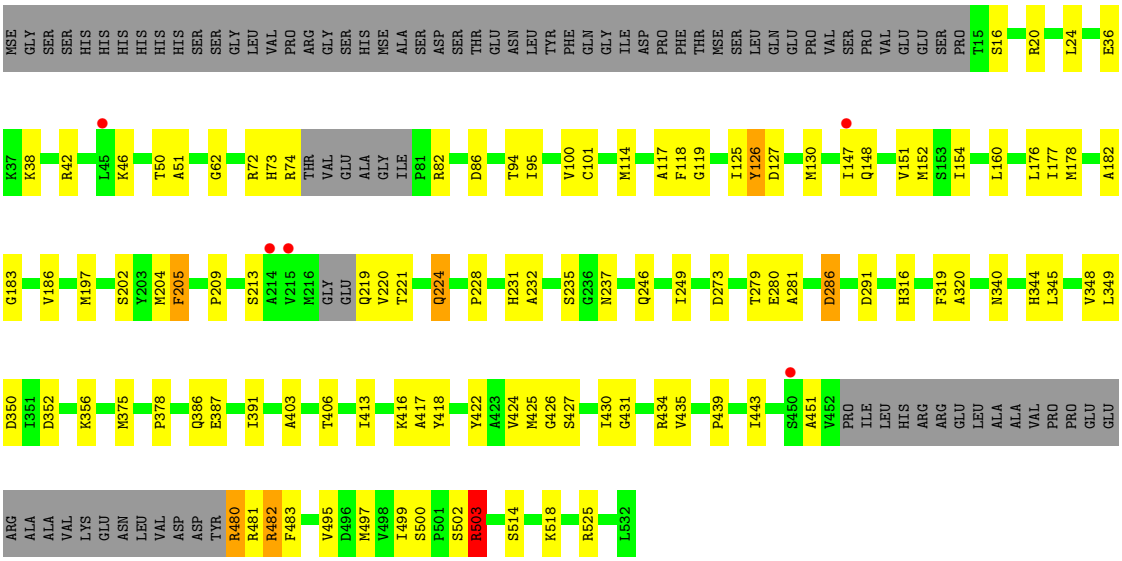


• Molecule 1: Putative carboxyl transferase



• Molecule 1: Putative carboxyl transferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	120.56Å 163.44Å 186.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.72 – 2.45 81.72 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (81.72-2.45) 90.2 (81.72-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.191 , 0.230 0.192 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	23360	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.39	2/3826 (0.1%)	0.60	1/5179 (0.0%)
1	B	0.35	0/3829	0.58	1/5184 (0.0%)
1	C	0.45	2/3872 (0.1%)	0.71	8/5242 (0.2%)
1	D	0.35	0/3765	0.58	1/5095 (0.0%)
1	E	0.41	1/3800 (0.0%)	0.63	2/5143 (0.0%)
1	F	0.41	1/3722 (0.0%)	0.67	5/5033 (0.1%)
All	All	0.39	6/22814 (0.0%)	0.63	18/30876 (0.1%)

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	C	0	1
1	E	0	2
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	GLU	CD-OE1	-7.00	1.18	1.25
1	C	473	GLU	CB-CG	-6.69	1.39	1.52
1	F	503	ARG	CG-CD	6.61	1.68	1.51
1	E	293	GLU	CG-CD	-5.83	1.43	1.51
1	A	210	GLU	CD-OE2	-5.82	1.19	1.25
1	C	479	TYR	CB-CG	-5.07	1.44	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	450	SER	CB-CA-C	-13.28	84.87	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	480	ARG	NE-CZ-NH1	-8.87	115.86	120.30
1	C	78	ALA	CB-CA-C	-8.71	97.04	110.10
1	F	503	ARG	CG-CD-NE	8.24	129.10	111.80
1	F	147	ILE	CG1-CB-CG2	7.75	128.44	111.40
1	E	298	ASP	CB-CG-OD1	6.87	124.49	118.30
1	D	45	LEU	CA-CB-CG	-6.48	100.39	115.30
1	A	383	GLY	N-CA-C	6.33	128.92	113.10
1	B	147	ILE	CG1-CB-CG2	6.26	125.17	111.40
1	C	449	ASN	CB-CA-C	-5.71	98.99	110.40
1	F	46	LYS	CD-CE-NZ	5.48	124.30	111.70
1	C	479	TYR	CA-CB-CG	5.36	123.58	113.40
1	F	160	LEU	CA-CB-CG	-5.36	102.98	115.30
1	C	480	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	F	480	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	78	ALA	N-CA-C	5.21	125.07	111.00
1	E	293	GLU	OE1-CD-OE2	5.03	129.34	123.30
1	C	450	SER	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	VAL	Peptide
1	A	452	VAL	Peptide
1	C	450	SER	Peptide
1	E	217	GLY	Peptide
1	E	298	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3760	0	3697	63	0
1	B	3763	0	3703	66	0
1	C	3806	0	3747	116	1
1	D	3700	0	3641	74	0
1	E	3735	0	3669	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3660	0	3607	104	0
2	A	166	0	0	7	1
2	B	214	0	0	2	0
2	C	156	0	0	6	0
2	D	152	0	0	3	0
2	E	136	0	0	1	0
2	F	112	0	0	6	0
All	All	23360	0	22064	478	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (478) 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:C:293:GLU:CG	1:C:480:ARG:NH2	1.97	1.26
1:B:385:GLY:O	1:B:389:GLN:HG3	1.38	1.24
1:C:293:GLU:HG3	1:C:480:ARG:NH2	1.48	1.23
1:F:500:SER:N	1:F:503:ARG:HH21	1.47	1.10
1:F:482:ARG:H	1:F:482:ARG:HD3	1.20	1.06
1:C:472:LYS:HZ3	1:C:475:LEU:HD23	1.16	1.05
1:F:500:SER:H	1:F:503:ARG:NH2	1.54	1.04
1:C:293:GLU:HG2	1:C:480:ARG:NH2	1.71	1.03
1:C:293:GLU:HG2	1:C:480:ARG:CZ	1.88	1.03
1:F:221:THR:HG22	1:F:224:GLN:HG2	1.40	1.02
1:B:385:GLY:O	1:B:389:GLN:CG	2.07	1.02
1:C:114:MSE:HE3	1:C:156:TYR:HB3	1.38	1.01
1:D:221:THR:HG22	1:D:224:GLN:HG3	1.39	0.99
1:E:298:ASP:HB2	1:E:343:ARG:CZ	1.92	0.98
1:C:293:GLU:HG3	1:C:480:ARG:HH22	1.26	0.97
1:B:445:VAL:HA	1:F:154:ILE:HD11	1.46	0.94
1:C:472:LYS:NZ	1:C:475:LEU:HD23	1.83	0.93
1:C:293:GLU:CG	1:C:480:ARG:HH22	1.74	0.90
1:A:445:VAL:HA	1:D:154:ILE:HD11	1.52	0.90
1:C:199:LYS:NZ	2:C:601:HOH:O	2.04	0.90
1:E:213:SER:HB2	1:E:219:GLN:HA	1.54	0.90
1:F:500:SER:H	1:F:503:ARG:HH21	0.94	0.89
1:B:434:ARG:HD2	1:B:497:MSE:HE3	1.51	0.89
1:F:221:THR:N	2:F:601:HOH:O	2.08	0.86
1:F:434:ARG:HD2	1:F:497:MSE:HE3	1.57	0.86
1:D:438:TRP:CZ2	1:D:504:THR:HG21	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:TRP:HZ2	1:D:504:THR:HG21	1.41	0.85
1:A:299:MSE:HE3	1:A:374:PHE:HB3	1.58	0.84
1:E:375:MSE:HE1	1:E:422:TYR:HD1	1.42	0.84
1:B:299:MSE:HE1	1:B:414:THR:HG21	1.61	0.82
1:E:88:VAL:O	1:E:121:LYS:NZ	2.12	0.82
1:C:451:ALA:O	1:C:452:VAL:HG13	1.81	0.81
1:F:127:ASP:HA	1:F:130:MSE:HE2	1.61	0.81
1:C:375:MSE:HE1	1:C:422:TYR:HA	1.62	0.80
1:C:293:GLU:N	1:C:293:GLU:OE2	2.16	0.79
1:D:479:TYR:N	2:D:601:HOH:O	2.16	0.78
1:E:298:ASP:OD1	1:E:341:GLN:NE2	2.15	0.78
1:A:139:ILE:HG23	1:A:178:MSE:HE3	1.65	0.77
1:C:293:GLU:O	1:C:415:ARG:NH2	2.17	0.77
1:E:33:VAL:HG13	1:E:34:LEU:HD12	1.67	0.77
1:A:375:MSE:HE1	1:A:422:TYR:HD1	1.49	0.77
1:C:471:VAL:HG13	1:C:472:LYS:H	1.50	0.77
1:C:375:MSE:HE2	1:C:417:ALA:HA	1.66	0.77
1:B:114:MSE:HE1	1:B:119:GLY:HA3	1.66	0.77
1:C:116:GLU:OE1	1:D:74:ARG:NH2	2.18	0.76
1:C:221:THR:HG23	1:C:224:GLN:H	1.51	0.75
1:B:20:ARG:NH2	1:C:484:GLY:O	2.20	0.75
1:C:473:GLU:N	1:C:473:GLU:OE2	2.19	0.74
1:C:199:LYS:HZ2	1:C:200:ASP:H	1.35	0.74
1:A:475:LEU:N	2:A:603:HOH:O	2.21	0.74
1:C:477:ASP:O	1:C:479:TYR:N	2.21	0.73
1:F:500:SER:H	1:F:503:ARG:CZ	2.02	0.73
1:B:147:ILE:HD11	1:F:451:ALA:HB1	1.68	0.73
1:A:434:ARG:HD2	1:A:497:MSE:HE3	1.71	0.72
1:B:114:MSE:HE2	1:B:156:TYR:HB3	1.71	0.72
1:B:114:MSE:HE1	1:B:119:GLY:CA	2.20	0.72
1:A:311:ASP:OD1	2:A:601:HOH:O	2.08	0.71
1:C:74:ARG:NH2	1:D:116:GLU:OE2	2.20	0.70
1:D:220:VAL:HG23	1:D:224:GLN:HB2	1.73	0.70
1:F:500:SER:N	1:F:503:ARG:NH2	2.25	0.69
1:C:478:ASP:HB3	1:C:481:ARG:HD2	1.74	0.69
1:F:482:ARG:HD3	1:F:482:ARG:N	2.03	0.69
1:C:204:MSE:HE2	1:E:392:ILE:HD13	1.75	0.69
1:F:417:ALA:HB3	1:F:443:ILE:HA	1.74	0.68
1:D:481:ARG:H	1:D:481:ARG:HD2	1.58	0.68
1:E:80:ILE:HD12	1:E:81:PRO:HD2	1.75	0.68
1:B:52:ARG:NH2	1:B:66:GLU:OE2	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:HB3	1:C:152:MSE:CE	2.23	0.67
1:E:378:PRO:HB3	1:E:416:LYS:HD2	1.77	0.67
1:C:471:VAL:HG13	1:C:472:LYS:N	2.09	0.67
1:C:445:VAL:HA	1:E:154:ILE:HD11	1.77	0.67
1:E:208:GLY:O	1:E:212:VAL:HG23	1.95	0.67
1:C:246:GLN:OE1	2:C:602:HOH:O	2.13	0.66
1:F:499:ILE:HA	1:F:503:ARG:NH2	2.09	0.66
1:D:215:VAL:HG12	1:D:216:MSE:HE3	1.78	0.66
1:D:272:HIS:NE2	1:D:274:CYS:HB2	2.10	0.66
1:C:293:GLU:HG2	1:C:480:ARG:NH1	2.10	0.66
1:B:114:MSE:HE2	1:B:156:TYR:CB	2.26	0.65
1:B:503:ARG:NH2	1:B:507:GLU:OE1	2.28	0.65
1:F:480:ARG:N	2:F:605:HOH:O	2.29	0.65
1:A:382:PRO:O	2:A:602:HOH:O	2.13	0.65
1:E:316:HIS:CB	1:E:356:LYS:HE3	2.26	0.65
1:C:476:VAL:O	1:C:478:ASP:N	2.29	0.65
1:A:375:MSE:HE1	1:A:422:TYR:CD1	2.31	0.64
1:B:130:MSE:HE1	1:B:163:ARG:HG2	1.79	0.64
1:C:199:LYS:NZ	1:C:200:ASP:H	1.94	0.64
1:A:323:ILE:O	1:A:356:LYS:NZ	2.30	0.64
1:C:436:MSE:HE3	1:C:507:GLU:HB2	1.77	0.64
1:C:375:MSE:CE	1:C:422:TYR:HA	2.27	0.64
1:E:298:ASP:OD2	1:E:300:ALA:HB3	1.97	0.64
1:B:405:SER:OG	1:B:409:LYS:HE3	1.98	0.64
1:C:449:ASN:C	1:C:449:ASN:OD1	2.36	0.64
1:E:24:LEU:HD21	1:F:503:ARG:NH2	2.13	0.63
1:F:114:MSE:HE3	1:F:118:PHE:CD1	2.34	0.63
1:E:375:MSE:HE1	1:E:422:TYR:CD1	2.30	0.62
1:C:114:MSE:HE3	1:C:156:TYR:CB	2.25	0.61
1:D:285:LEU:HA	1:D:288:VAL:HG13	1.81	0.61
1:D:373:THR:HB	1:D:411:THR:HG23	1.83	0.61
1:F:406:THR:O	1:F:518:LYS:HE2	1.99	0.61
1:F:126:TYR:O	1:F:130:MSE:HG3	2.01	0.61
1:D:272:HIS:CE1	1:D:331:GLU:HA	2.36	0.61
1:C:429:GLN:OE1	2:C:603:HOH:O	2.16	0.61
1:A:15:THR:HG22	1:B:481:ARG:HH22	1.65	0.61
1:A:197:MSE:HE3	1:A:238:ALA:HB2	1.82	0.60
1:F:480:ARG:HG2	1:F:482:ARG:NH1	2.16	0.60
1:F:114:MSE:HE3	1:F:118:PHE:HD1	1.65	0.60
1:C:148:GLN:OE1	1:C:148:GLN:N	2.29	0.60
1:C:472:LYS:HZ3	1:C:475:LEU:CD2	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:TYR:CE2	1:E:136:VAL:HG11	2.37	0.60
1:F:72:ARG:HB2	1:F:82:ARG:HH21	1.66	0.60
1:C:476:VAL:C	1:C:478:ASP:H	2.03	0.60
1:F:36:GLU:OE2	1:F:50:THR:HG21	2.01	0.60
1:F:500:SER:H	1:F:503:ARG:NE	1.99	0.60
1:C:183:GLY:O	1:C:186:VAL:HG22	2.02	0.59
1:F:316:HIS:HB2	1:F:356:LYS:HE3	1.83	0.59
1:C:293:GLU:CG	1:C:480:ARG:CZ	2.61	0.59
1:E:350:ASP:HB2	1:E:386:GLN:HE22	1.67	0.59
1:D:387:GLU:HA	1:D:391:ILE:HG22	1.85	0.59
1:F:316:HIS:CB	1:F:356:LYS:HE3	2.32	0.59
1:C:76:VAL:HA	1:C:82:ARG:HD2	1.84	0.58
1:F:500:SER:H	1:F:503:ARG:HE	1.50	0.58
1:A:375:MSE:HE2	1:A:413:ILE:HG12	1.85	0.58
1:E:316:HIS:HB2	1:E:356:LYS:HE3	1.84	0.58
1:B:16:SER:O	1:B:20:ARG:HG3	2.03	0.58
1:B:159:GLU:O	1:B:162:VAL:HG12	2.02	0.58
1:A:385:GLY:O	1:A:389:GLN:HG3	2.03	0.58
1:C:475:LEU:HG	1:C:475:LEU:O	2.03	0.58
1:D:438:TRP:HE1	1:D:504:THR:CG2	2.16	0.58
1:F:178:MSE:HE1	1:F:249:ILE:HG13	1.86	0.58
1:C:436:MSE:HG2	1:C:497:MSE:HE2	1.85	0.57
1:C:470:ALA:HA	1:C:473:GLU:OE1	2.03	0.57
1:C:213:SER:OG	1:C:218:GLU:O	2.15	0.57
1:E:299:MSE:HE3	1:E:302:VAL:HB	1.86	0.56
1:E:212:VAL:HG21	1:E:225:LEU:HD21	1.87	0.56
1:C:473:GLU:HG2	1:C:474:ASN:H	1.71	0.56
1:A:176:LEU:HB3	1:A:178:MSE:HE2	1.88	0.55
1:A:99:GLN:OE1	1:B:514:SER:HB2	2.05	0.55
1:B:197:MSE:SE	1:B:204:MSE:HE2	2.56	0.55
1:E:350:ASP:HB2	1:E:386:GLN:NE2	2.21	0.55
1:A:285:LEU:O	1:A:288:VAL:HG12	2.07	0.55
1:D:376:ASP:OD1	1:D:416:LYS:HE2	2.06	0.55
1:D:221:THR:HG23	1:D:223:GLU:H	1.70	0.55
1:B:30:GLU:HA	1:B:34:LEU:HD12	1.89	0.55
1:B:448:ALA:HA	1:B:479:TYR:CD2	2.42	0.55
1:B:506:TYR:CZ	1:B:510:ARG:HD2	2.42	0.55
1:E:139:ILE:HG12	1:E:176:LEU:HD12	1.87	0.55
1:E:316:HIS:HB3	1:E:356:LYS:HE3	1.88	0.55
1:E:381:LEU:HD12	1:E:382:PRO:HD2	1.88	0.54
1:A:146:ARG:HD2	1:A:149:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:GLU:HB3	1:C:152:MSE:HE3	1.89	0.54
1:F:151:VAL:HA	1:F:154:ILE:HD12	1.89	0.54
1:B:114:MSE:HE3	1:B:115:GLY:O	2.07	0.54
1:E:99:GLN:OE1	1:F:514:SER:HB2	2.07	0.54
1:F:481:ARG:H	1:F:482:ARG:NH2	2.06	0.54
1:F:482:ARG:H	1:F:482:ARG:CD	2.06	0.54
1:A:23:ASP:OD2	1:A:27:ARG:NH1	2.40	0.54
1:A:197:MSE:HE2	1:A:204:MSE:SE	2.57	0.54
1:E:351:ILE:H	1:E:386:GLN:HE22	1.54	0.53
1:F:500:SER:N	1:F:503:ARG:HE	2.06	0.53
1:B:148:GLN:H	1:B:148:GLN:CD	2.07	0.53
1:B:345:LEU:O	1:B:348:VAL:HG22	2.08	0.53
1:D:297:TYR:OH	1:D:376:ASP:OD2	2.21	0.53
1:D:510:ARG:NH2	1:F:62:GLY:O	2.42	0.53
1:E:298:ASP:CB	1:E:343:ARG:CZ	2.78	0.53
1:C:73:HIS:CE1	1:C:82:ARG:HG2	2.43	0.53
1:C:88:VAL:HB	1:C:118:PHE:CE2	2.44	0.53
1:E:298:ASP:CG	1:E:300:ALA:H	2.11	0.53
1:B:127:ASP:HA	1:B:130:MSE:HE3	1.91	0.53
1:E:293:GLU:OE1	1:E:480:ARG:NH1	2.42	0.53
1:F:197:MSE:HE3	1:F:204:MSE:HG3	1.91	0.53
1:F:340:ASN:HD21	1:F:425:MSE:HE2	1.74	0.53
1:F:16:SER:O	1:F:20:ARG:HG3	2.07	0.53
1:A:299:MSE:HE3	1:A:374:PHE:CB	2.37	0.53
1:F:340:ASN:ND2	1:F:425:MSE:HE2	2.24	0.53
1:C:41:ASP:O	1:C:45:LEU:HD13	2.09	0.52
1:C:473:GLU:HG2	1:C:474:ASN:N	2.25	0.52
1:C:285:LEU:O	1:C:288:VAL:HG12	2.09	0.52
1:B:43:GLN:HG2	1:B:49:LEU:O	2.09	0.52
1:C:479:TYR:CE2	1:C:483:PHE:CD2	2.97	0.52
1:A:23:ASP:O	1:A:27:ARG:HG3	2.09	0.52
1:D:52:ARG:HH22	1:D:66:GLU:CD	2.13	0.52
1:D:197:MSE:SE	1:D:204:MSE:HE2	2.60	0.52
1:F:197:MSE:SE	1:F:204:MSE:HE2	2.59	0.52
1:F:375:MSE:HE1	1:F:422:TYR:HD1	1.74	0.52
1:C:345:LEU:O	1:C:348:VAL:HG22	2.10	0.52
1:C:375:MSE:HE3	1:C:377:VAL:HG12	1.91	0.52
1:A:43:GLN:NE2	1:A:49:LEU:O	2.39	0.52
1:E:299:MSE:CE	1:E:302:VAL:HB	2.38	0.52
1:C:293:GLU:HG3	1:C:480:ARG:HH21	1.62	0.52
1:C:470:ALA:HA	1:C:473:GLU:CD	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:ARG:HD2	1:D:481:ARG:N	2.24	0.51
1:F:246:GLN:CD	1:F:246:GLN:H	2.14	0.51
1:E:375:MSE:SE	1:E:422:TYR:HA	2.61	0.51
1:E:507:GLU:OE1	1:E:507:GLU:HA	2.10	0.51
1:F:435:VAL:HG12	1:F:495:VAL:HG12	1.92	0.51
1:B:406:THR:O	1:B:518:LYS:HE2	2.10	0.51
1:C:316:HIS:HB2	1:C:356:LYS:HE2	1.92	0.51
1:F:350:ASP:HB2	1:F:386:GLN:HE22	1.75	0.51
1:F:220:VAL:CG1	1:F:224:GLN:HG3	2.41	0.51
1:F:220:VAL:HG13	1:F:224:GLN:HG3	1.93	0.51
1:B:52:ARG:HG3	2:B:705:HOH:O	2.11	0.51
1:E:88:VAL:HB	1:E:118:PHE:CE2	2.46	0.51
1:E:139:ILE:HG23	1:E:178:MSE:SE	2.61	0.51
1:A:88:VAL:HB	1:A:118:PHE:CE2	2.46	0.51
1:C:320:ALA:HB2	1:C:352:ASP:HB3	1.92	0.51
1:E:298:ASP:HB2	1:E:343:ARG:NH2	2.24	0.51
1:F:101:CYS:HB3	1:F:125:ILE:HG23	1.93	0.51
1:B:385:GLY:O	1:B:389:GLN:HG2	2.04	0.50
1:A:152:MSE:HE3	1:D:492:HIS:CE1	2.46	0.50
1:E:24:LEU:HD21	1:F:503:ARG:HH22	1.76	0.50
1:E:33:VAL:CG1	1:E:34:LEU:HD12	2.41	0.50
1:A:117:ALA:O	1:A:121:LYS:HG3	2.12	0.50
1:B:433:ASP:OD1	1:B:518:LYS:NZ	2.36	0.50
1:D:316:HIS:HB3	1:D:356:LYS:HE3	1.93	0.50
1:D:68:ASP:CB	1:D:121:LYS:HD2	2.42	0.50
1:D:176:LEU:HD23	1:D:196:VAL:HB	1.93	0.50
1:D:323:ILE:O	1:D:356:LYS:NZ	2.44	0.50
1:C:375:MSE:HE1	1:C:422:TYR:CA	2.36	0.50
1:D:506:TYR:CE2	1:D:510:ARG:HD2	2.47	0.50
1:C:116:GLU:HB3	1:C:152:MSE:HE1	1.91	0.50
1:C:231:HIS:CD2	1:C:237:ASN:HD22	2.30	0.50
1:D:499:ILE:HG22	2:D:603:HOH:O	2.12	0.50
1:C:86:ASP:OD2	1:C:117:ALA:HB3	2.12	0.49
1:F:500:SER:HB3	1:F:503:ARG:NE	2.27	0.49
1:F:38:LYS:O	1:F:42:ARG:HG3	2.12	0.49
1:B:497:MSE:HE1	2:B:611:HOH:O	2.12	0.49
1:D:427:SER:O	1:D:430:ILE:HG22	2.12	0.49
1:A:116:GLU:OE2	1:F:74:ARG:NH2	2.43	0.49
1:D:481:ARG:NH2	2:D:601:HOH:O	2.21	0.49
1:E:136:VAL:HG23	1:E:171:ILE:HD12	1.95	0.49
1:E:183:GLY:O	1:E:186:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:220:VAL:HG21	1:E:225:LEU:HD13	1.95	0.49
1:B:43:GLN:HG3	1:B:48:LYS:HB2	1.93	0.49
1:F:427:SER:O	1:F:430:ILE:HG22	2.12	0.49
1:D:99:GLN:OE1	1:E:514:SER:HB2	2.13	0.49
1:A:38:LYS:HD2	1:A:38:LYS:C	2.33	0.48
1:D:16:SER:O	1:D:20:ARG:HG3	2.13	0.48
1:F:480:ARG:HD2	1:F:483:PHE:HD2	1.78	0.48
1:E:23:ASP:O	1:E:27:ARG:HG3	2.12	0.48
1:F:500:SER:HB3	1:F:503:ARG:HE	1.78	0.48
1:A:206:VAL:N	1:D:387:GLU:OE2	2.42	0.48
1:D:71:VAL:HB	1:D:121:LYS:HD3	1.95	0.48
1:D:439:PRO:HD3	1:D:499:ILE:O	2.13	0.48
1:D:342:PRO:HA	1:D:347:GLY:N	2.28	0.48
1:F:319:PHE:O	1:F:356:LYS:NZ	2.30	0.48
1:C:204:MSE:HB2	1:C:231:HIS:CE1	2.48	0.48
1:E:497:MSE:HG2	1:E:499:ILE:HG23	1.95	0.48
1:A:28:HIS:CE1	1:A:32:VAL:HG21	2.49	0.48
1:D:29:GLU:OE2	1:D:34:LEU:HD21	2.14	0.48
1:D:125:ILE:HD12	1:D:125:ILE:HA	1.80	0.48
1:B:177:ILE:HB	1:B:197:MSE:HG2	1.96	0.47
1:C:375:MSE:CE	1:C:417:ALA:HA	2.41	0.47
1:B:178:MSE:HE1	1:B:249:ILE:HG13	1.96	0.47
1:E:43:GLN:NE2	1:E:49:LEU:O	2.44	0.47
1:E:231:HIS:HA	1:E:235:SER:OG	2.14	0.47
1:E:338:VAL:O	1:E:373:THR:HA	2.14	0.47
1:F:387:GLU:HA	1:F:391:ILE:HG22	1.96	0.47
1:B:43:GLN:HG3	1:B:48:LYS:CB	2.44	0.47
1:B:438:TRP:CZ2	1:B:501:PRO:HB3	2.49	0.47
1:D:181:CYS:O	1:D:204:MSE:HA	2.14	0.47
1:F:273:ASP:OD1	1:F:273:ASP:N	2.47	0.47
1:A:445:VAL:HG13	1:A:446:MSE:HG2	1.96	0.47
1:B:126:TYR:O	1:B:130:MSE:HG3	2.14	0.47
1:C:43:GLN:OE1	1:C:48:LYS:HE2	2.15	0.47
1:A:159:GLU:OE1	1:A:163:ARG:NH1	2.47	0.47
1:C:436:MSE:CE	1:C:504:THR:HA	2.44	0.47
1:D:68:ASP:HB2	1:D:121:LYS:HD2	1.97	0.47
1:A:126:TYR:CE2	1:A:136:VAL:HG11	2.50	0.47
1:B:506:TYR:CE2	1:B:510:ARG:HD2	2.49	0.47
1:D:495:VAL:HG12	1:D:497:MSE:H	1.77	0.47
1:E:86:ASP:OD2	1:E:117:ALA:HB3	2.14	0.47
1:F:320:ALA:HB2	1:F:352:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ALA:HB2	1:A:352:ASP:HB3	1.96	0.47
1:B:316:HIS:HB3	1:B:356:LYS:HE3	1.97	0.47
1:C:497:MSE:HE3	1:C:499:ILE:HG21	1.97	0.47
1:F:375:MSE:HE1	1:F:422:TYR:CD1	2.50	0.47
1:A:375:MSE:HE3	1:A:417:ALA:HB2	1.97	0.47
1:B:435:VAL:HG12	1:B:495:VAL:HG12	1.96	0.47
1:D:428:ARG:HH21	1:D:496:ASP:CG	2.16	0.47
1:B:320:ALA:HB2	1:B:352:ASP:HB3	1.96	0.46
1:F:375:MSE:HE2	1:F:413:ILE:HG23	1.97	0.46
1:A:95:ILE:HG13	1:A:100:VAL:HG21	1.97	0.46
1:A:293:GLU:HA	1:A:415:ARG:NH2	2.30	0.46
1:D:316:HIS:CB	1:D:356:LYS:HE3	2.45	0.46
1:F:73:HIS:CE1	1:F:82:ARG:HG2	2.50	0.46
1:A:220:VAL:HG22	1:A:224:GLN:HB2	1.97	0.46
1:F:386:GLN:NE2	2:F:603:HOH:O	2.26	0.46
1:C:29:GLU:CD	1:C:33:VAL:HG21	2.36	0.46
1:C:74:ARG:HG3	1:C:116:GLU:OE1	2.15	0.46
1:F:183:GLY:O	1:F:186:VAL:HG22	2.16	0.46
1:F:279:THR:HG22	1:F:281:ALA:H	1.80	0.46
1:C:220:VAL:HG22	1:C:224:GLN:HB2	1.97	0.46
1:C:473:GLU:O	1:C:476:VAL:HG22	2.15	0.46
1:D:104:SER:HA	1:D:139:ILE:HB	1.98	0.46
1:F:481:ARG:H	1:F:482:ARG:HH21	1.62	0.46
1:B:23:ASP:O	1:B:27:ARG:HG3	2.16	0.46
1:A:249:ILE:O	1:A:253:GLN:HG3	2.16	0.46
1:D:62:GLY:O	1:E:510:ARG:NH2	2.49	0.46
1:B:99:GLN:OE1	1:C:514:SER:HB2	2.16	0.46
1:C:439:PRO:HD3	1:C:499:ILE:O	2.15	0.46
1:D:272:HIS:NE2	1:D:331:GLU:HA	2.30	0.46
1:C:242:GLY:HA2	1:C:247:ASP:OD2	2.16	0.46
1:C:472:LYS:HZ1	1:C:476:VAL:HG12	1.79	0.46
1:C:473:GLU:C	1:C:475:LEU:H	2.20	0.46
1:D:220:VAL:CG2	1:D:224:GLN:HB2	2.42	0.46
1:E:244:ASP:OD1	1:E:247:ASP:N	2.39	0.46
1:E:387:GLU:HA	1:E:391:ILE:HG22	1.97	0.46
1:C:392:ILE:HD13	1:E:206:VAL:HG23	1.96	0.45
1:F:286:ASP:OD1	1:F:502:SER:HB3	2.15	0.45
1:A:68:ASP:HB2	1:A:121:LYS:HE3	1.99	0.45
1:C:117:ALA:O	1:C:121:LYS:HG3	2.17	0.45
1:F:204:MSE:HB2	1:F:231:HIS:CE1	2.51	0.45
1:C:231:HIS:HA	1:C:235:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ASP:OD1	1:C:416:LYS:HB2	2.17	0.45
1:F:177:ILE:HB	1:F:197:MSE:HG2	1.97	0.45
1:A:448:ALA:O	1:A:476:VAL:HG22	2.17	0.45
1:E:82:ARG:O	1:E:82:ARG:CG	2.65	0.45
1:B:448:ALA:HA	1:B:479:TYR:CE2	2.51	0.45
1:D:221:THR:HG23	1:D:223:GLU:N	2.31	0.45
1:E:249:ILE:O	1:E:253:GLN:HG3	2.17	0.45
1:F:86:ASP:OD2	1:F:117:ALA:HB3	2.17	0.45
1:F:439:PRO:HD3	1:F:499:ILE:O	2.17	0.45
1:B:117:ALA:O	1:B:121:LYS:HG3	2.17	0.45
1:C:44:HIS:HE1	2:C:718:HOH:O	1.99	0.45
1:F:231:HIS:HD2	1:F:235:SER:OG	2.00	0.45
1:F:431:GLY:HA3	2:F:686:HOH:O	2.16	0.45
1:C:221:THR:HG22	1:C:224:GLN:OE1	2.17	0.45
1:D:437:ALA:O	1:D:498:VAL:HA	2.16	0.45
1:E:202:SER:O	1:E:228:PRO:HD3	2.17	0.45
1:C:471:VAL:CG1	1:C:472:LYS:N	2.79	0.45
1:F:350:ASP:HB2	1:F:386:GLN:NE2	2.32	0.45
1:A:73:HIS:CE1	1:A:82:ARG:HG2	2.52	0.45
1:B:213:SER:HB2	1:B:219:GLN:OE1	2.17	0.45
1:C:344:HIS:ND1	1:C:345:LEU:HG	2.32	0.45
1:C:471:VAL:CG1	1:C:472:LYS:H	2.25	0.45
1:C:436:MSE:HE1	1:C:504:THR:HA	1.99	0.44
1:A:183:GLY:O	1:A:186:VAL:HG22	2.17	0.44
1:A:446:MSE:SE	1:D:147:ILE:HD11	2.66	0.44
1:C:29:GLU:HA	1:C:33:VAL:HG22	1.99	0.44
1:E:285:LEU:O	1:E:288:VAL:HG12	2.17	0.44
1:C:48:LYS:NZ	1:C:141:ASP:OD1	2.44	0.44
1:C:48:LYS:NZ	2:C:610:HOH:O	2.44	0.44
1:C:477:ASP:OD1	1:C:477:ASP:C	2.56	0.44
1:F:344:HIS:ND1	1:F:345:LEU:HG	2.32	0.44
1:F:50:THR:HG22	1:F:51:ALA:N	2.32	0.44
1:F:424:VAL:O	1:F:426:GLY:N	2.49	0.44
1:A:199:LYS:O	1:A:228:PRO:HG2	2.18	0.44
1:C:438:TRP:N	1:C:438:TRP:CD1	2.83	0.44
1:D:338:VAL:O	1:D:373:THR:HA	2.18	0.44
1:D:45:LEU:HD23	1:D:45:LEU:HA	1.62	0.44
1:E:104:SER:HA	1:E:139:ILE:HB	2.00	0.44
1:E:251:TRP:CD1	1:E:313:LEU:HD11	2.53	0.44
1:D:249:ILE:O	1:D:253:GLN:HG3	2.18	0.44
1:E:329:ARG:HA	1:E:333:HIS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:LEU:HD22	1:F:178:MSE:HE3	2.00	0.44
1:B:439:PRO:HD3	1:B:499:ILE:O	2.17	0.44
1:E:205:PHE:CZ	1:E:209:PRO:HD3	2.53	0.44
1:E:298:ASP:OD1	1:E:343:ARG:HD2	2.18	0.44
1:E:427:SER:O	1:E:430:ILE:HG22	2.18	0.44
1:A:329:ARG:HA	1:A:333:HIS:O	2.18	0.44
1:D:88:VAL:HB	1:D:118:PHE:CE2	2.52	0.44
1:E:361:ILE:HD12	1:E:398:LEU:HD11	2.00	0.44
1:F:416:LYS:HD2	1:F:418:TYR:CZ	2.53	0.44
1:B:316:HIS:HB2	1:B:356:LYS:HE2	2.00	0.43
1:C:29:GLU:OE1	1:C:33:VAL:HG21	2.18	0.43
1:C:375:MSE:HE3	1:C:377:VAL:CG1	2.48	0.43
1:D:272:HIS:CE1	1:D:274:CYS:SG	3.11	0.43
1:E:16:SER:HB2	1:F:291:ASP:OD1	2.18	0.43
1:E:181:CYS:O	1:E:204:MSE:HA	2.18	0.43
1:F:114:MSE:CE	1:F:119:GLY:HA2	2.48	0.43
1:A:16:SER:O	1:A:20:ARG:HG3	2.18	0.43
1:B:86:ASP:OD2	1:B:117:ALA:HB3	2.19	0.43
1:D:438:TRP:CE2	1:D:504:THR:HG21	2.53	0.43
1:D:272:HIS:CD2	1:D:331:GLU:HA	2.53	0.43
1:A:116:GLU:CD	1:F:74:ARG:HH22	2.21	0.43
1:C:436:MSE:HE2	1:C:499:ILE:HD11	2.00	0.43
1:F:202:SER:O	1:F:228:PRO:HD3	2.18	0.43
1:B:162:VAL:HG23	1:F:403:ALA:HB1	1.99	0.43
1:F:279:THR:HG22	1:F:280:GLU:N	2.33	0.43
1:F:349:LEU:HD11	1:F:425:MSE:SE	2.69	0.43
1:B:285:LEU:HD21	1:B:302:VAL:HA	2.00	0.43
1:E:381:LEU:HD12	1:E:382:PRO:CD	2.49	0.43
1:A:71:VAL:HA	1:B:491:ALA:HA	2.01	0.43
1:C:38:LYS:HE3	1:C:38:LYS:HB3	1.74	0.43
1:C:378:PRO:HB3	1:C:416:LYS:HD2	1.99	0.43
1:E:147:ILE:HD12	1:E:147:ILE:H	1.83	0.43
1:E:299:MSE:HG2	1:E:339:ALA:HB1	2.01	0.43
1:F:204:MSE:O	1:F:231:HIS:HE1	2.02	0.43
1:A:72:ARG:HB2	1:A:82:ARG:HH21	1.83	0.43
1:B:74:ARG:HG3	1:B:116:GLU:OE1	2.18	0.43
1:E:72:ARG:CZ	1:E:82:ARG:HE	2.32	0.43
1:E:293:GLU:OE2	1:E:480:ARG:CZ	2.67	0.43
1:B:338:VAL:O	1:B:373:THR:HA	2.19	0.43
1:D:231:HIS:HA	1:D:235:SER:OG	2.19	0.43
1:F:375:MSE:SE	1:F:422:TYR:HA	2.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASP:HB2	1:B:386:GLN:OE1	2.18	0.42
1:C:338:VAL:HG12	1:C:425:MSE:HE1	2.01	0.42
1:D:197:MSE:HE3	1:D:204:MSE:HG3	2.01	0.42
1:D:375:MSE:HE2	1:D:425:MSE:O	2.19	0.42
1:A:71:VAL:CG1	1:A:117:ALA:HB1	2.49	0.42
1:A:321:ARG:NH1	2:A:613:HOH:O	2.50	0.42
1:D:179:GLY:HA2	1:D:201:ILE:O	2.19	0.42
1:D:439:PRO:HG3	1:F:24:LEU:HD22	2.01	0.42
1:F:348:VAL:HG12	1:F:378:PRO:HG2	2.01	0.42
1:A:359:ARG:HD3	2:A:636:HOH:O	2.20	0.42
1:A:505:ARG:NH2	2:A:618:HOH:O	2.52	0.42
1:D:501:PRO:O	1:D:504:THR:HG23	2.19	0.42
1:F:499:ILE:CA	1:F:503:ARG:NH2	2.80	0.42
1:C:348:VAL:CG1	1:C:378:PRO:HG2	2.49	0.42
1:E:439:PRO:HD3	1:E:499:ILE:O	2.19	0.42
1:F:221:THR:HB	2:F:601:HOH:O	2.18	0.42
1:A:416:LYS:HD2	1:A:418:TYR:CZ	2.54	0.42
1:B:38:LYS:HE3	1:B:38:LYS:HB3	1.82	0.42
1:C:316:HIS:HB3	1:C:356:LYS:HE3	2.01	0.42
1:C:417:ALA:HB3	1:C:443:ILE:HA	2.01	0.42
1:C:497:MSE:HE1	1:C:507:GLU:CG	2.50	0.42
1:A:417:ALA:HB3	1:A:443:ILE:HA	2.02	0.42
1:B:215:VAL:HG12	1:B:216:MSE:CE	2.50	0.42
1:C:338:VAL:O	1:C:373:THR:HA	2.20	0.42
1:C:244:ASP:HB2	2:C:602:HOH:O	2.20	0.42
1:C:472:LYS:O	1:C:476:VAL:HG13	2.20	0.42
1:E:299:MSE:HE3	1:E:299:MSE:O	2.20	0.42
1:E:358:ALA:O	1:E:362:ARG:HG3	2.20	0.42
1:C:68:ASP:OD2	1:C:124:LYS:HE3	2.19	0.41
1:D:88:VAL:HG13	1:D:121:LYS:HE3	2.02	0.41
1:D:198:VAL:HG12	1:D:201:ILE:HG12	2.02	0.41
1:E:299:MSE:HG2	1:E:340:ASN:O	2.20	0.41
1:E:322:ASN:OD1	1:E:322:ASN:N	2.52	0.41
1:F:95:ILE:HG13	1:F:100:VAL:HG21	2.01	0.41
1:F:205:PHE:CZ	1:F:209:PRO:HD3	2.55	0.41
1:F:316:HIS:HB3	1:F:356:LYS:HE3	2.00	0.41
1:A:338:VAL:O	1:A:373:THR:HA	2.19	0.41
1:F:213:SER:HB3	1:F:219:GLN:HA	2.02	0.41
1:F:435:VAL:CG1	1:F:495:VAL:HG12	2.50	0.41
1:B:242:GLY:HA2	1:B:247:ASP:OD2	2.20	0.41
1:D:438:TRP:HE1	1:D:504:THR:HG22	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:HIS:HA	1:F:235:SER:OG	2.21	0.41
1:F:480:ARG:HA	1:F:482:ARG:NH2	2.36	0.41
1:A:376:ASP:OD1	1:A:415:ARG:HB3	2.20	0.41
1:E:436:MSE:HE2	1:E:497:MSE:SE	2.69	0.41
1:C:148:GLN:H	1:C:148:GLN:CD	2.19	0.41
1:C:436:MSE:CE	1:C:507:GLU:HB2	2.49	0.41
1:D:23:ASP:O	1:D:27:ARG:HG3	2.20	0.41
1:D:77:GLU:HB2	1:D:80:ILE:HG13	2.02	0.41
1:B:289:ILE:HD11	1:B:438:TRP:HZ3	1.86	0.41
1:E:151:VAL:HA	1:E:154:ILE:HD12	2.01	0.41
1:A:86:ASP:OD2	1:A:117:ALA:HB3	2.21	0.41
1:D:202:SER:O	1:D:228:PRO:HD3	2.21	0.41
1:F:148:GLN:H	1:F:148:GLN:CD	2.13	0.41
1:A:298:ASP:HB2	1:A:343:ARG:HD2	2.03	0.41
1:C:231:HIS:HD2	1:C:237:ASN:HD22	1.68	0.41
1:C:427:SER:O	1:C:430:ILE:HG22	2.21	0.41
1:B:307:LEU:HD11	1:B:337:VAL:HG21	2.02	0.41
1:D:424:VAL:O	1:D:426:GLY:N	2.48	0.41
1:E:298:ASP:HB3	1:E:301:ASP:H	1.86	0.41
1:F:125:ILE:HD13	1:F:125:ILE:HA	1.81	0.41
1:F:525:ARG:NH2	2:F:616:HOH:O	2.51	0.41
1:C:141:ASP:OD1	1:C:179:GLY:HA3	2.21	0.41
1:E:74:ARG:HD3	1:E:116:GLU:OE2	2.21	0.41
1:E:299:MSE:CG	1:E:339:ALA:HB1	2.51	0.41
1:F:231:HIS:CD2	1:F:237:ASN:HD22	2.39	0.41
1:A:15:THR:HG22	1:B:481:ARG:NH2	2.32	0.40
1:C:497:MSE:HE1	1:C:507:GLU:HG3	2.03	0.40
1:A:140:ASN:ND2	2:A:605:HOH:O	2.31	0.40
1:B:358:ALA:O	1:B:362:ARG:HG3	2.21	0.40
1:B:416:LYS:HD2	1:B:418:TYR:CZ	2.56	0.40
1:C:221:THR:HG22	1:C:224:GLN:HG3	2.03	0.40
1:E:251:TRP:NE1	1:E:313:LEU:HD11	2.35	0.40
1:F:182:ALA:HA	1:F:205:PHE:O	2.21	0.40
1:F:232:ALA:O	1:F:319:PHE:HB2	2.21	0.40
1:E:213:SER:HA	1:E:218:GLU:O	2.22	0.40
1:A:381:LEU:HA	1:A:382:PRO:HD3	1.79	0.40
1:C:226:GLY:O	1:C:231:HIS:CE1	2.75	0.40
1:D:52:ARG:NH2	1:D:66:GLU:OE2	2.55	0.40
1:B:114:MSE:HE2	1:B:156:TYR:HB2	2.01	0.40
1:D:438:TRP:NE1	1:D:504:THR:CG2	2.84	0.40
1:E:29:GLU:O	1:E:33:VAL:HG12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:ARG:NH1	2:E:617:HOH:O	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ALA:N	2:A:764:HOH:O[1_655]	2.02	0.18

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	490/570 (86%)	470 (96%)	18 (4%)	2 (0%)	34 41
1	B	493/570 (86%)	478 (97%)	15 (3%)	0	100 100
1	C	499/570 (88%)	480 (96%)	16 (3%)	3 (1%)	25 29
1	D	484/570 (85%)	467 (96%)	17 (4%)	0	100 100
1	E	485/570 (85%)	469 (97%)	15 (3%)	1 (0%)	47 57
1	F	475/570 (83%)	459 (97%)	16 (3%)	0	100 100
All	All	2926/3420 (86%)	2823 (96%)	97 (3%)	6 (0%)	47 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	477	ASP
1	C	478	ASP
1	A	383	GLY
1	C	474	ASN
1	A	452	VAL
1	E	141	ASP

5.3.2 Protein sidechains (i)

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	395/442 (89%)	389 (98%)	6 (2%)	65	76
1	B	394/442 (89%)	388 (98%)	6 (2%)	65	76
1	C	398/442 (90%)	393 (99%)	5 (1%)	69	79
1	D	386/442 (87%)	383 (99%)	3 (1%)	81	88
1	E	391/442 (88%)	388 (99%)	3 (1%)	81	88
1	F	383/442 (87%)	375 (98%)	8 (2%)	53	66
All	All	2347/2652 (88%)	2316 (99%)	31 (1%)	69	79

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	126	TYR
1	A	148	GLN
1	A	205	PHE
1	A	219	GLN
1	A	299	MSE
1	B	38	LYS
1	B	126	TYR
1	B	409	LYS
1	B	445	VAL
1	B	452	VAL
1	B	477	ASP
1	C	178	MSE
1	C	450	SER
1	C	475	LEU
1	C	482	ARG
1	C	519	ARG
1	D	126	TYR
1	D	481	ARG
1	D	500	SER
1	E	126	TYR
1	E	299	MSE

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Mol	Chain	Res	Type
1	E	388	HIS
1	F	94	THR
1	F	126	TYR
1	F	152	MSE
1	F	205	PHE
1	F	224	GLN
1	F	286	ASP
1	F	482	ARG
1	F	503	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	164	ASN
1	C	231	HIS
1	E	386	GLN
1	F	231	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 monosaccharides 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^{th} 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^2)	Q<0.9
1	A	483/570 (84%)	-0.05	7 (1%)	75 74	25, 42, 77, 104	0
1	B	484/570 (84%)	-0.12	12 (2%)	57 53	23, 39, 73, 112	0
1	C	490/570 (85%)	-0.07	16 (3%)	46 43	25, 41, 89, 141	0
1	D	475/570 (83%)	-0.05	9 (1%)	66 64	25, 45, 78, 130	0
1	E	481/570 (84%)	0.17	25 (5%)	27 24	27, 50, 85, 112	0
1	F	470/570 (82%)	-0.04	5 (1%)	80 80	28, 50, 80, 102	0
All	All	2883/3420 (84%)	-0.03	74 (2%)	56 52	23, 44, 81, 141	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	76	VAL	6.2
1	D	294	GLN	5.6
1	C	214	ALA	5.1
1	C	474	ASN	5.0
1	E	476	VAL	4.9
1	E	475	LEU	4.6
1	C	470	ALA	4.6
1	B	78	ALA	4.5
1	E	14	PRO	4.5
1	C	479	TYR	4.3
1	D	479	TYR	4.0
1	D	76	VAL	4.0
1	C	215	VAL	3.9
1	E	479	TYR	3.5
1	B	14	PRO	3.5
1	C	471	VAL	3.4
1	A	215	VAL	3.4
1	E	80	ILE	3.2
1	E	76	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	476	VAL	3.2
1	D	78	ALA	3.1
1	E	481	ARG	3.1
1	A	214	ALA	3.1
1	B	479	TYR	3.0
1	F	215	VAL	3.0
1	E	343	ARG	2.9
1	E	212	VAL	2.8
1	C	473	GLU	2.8
1	E	15	THR	2.8
1	F	147	ILE	2.7
1	F	214	ALA	2.7
1	C	294	GLN	2.7
1	C	210	GLU	2.7
1	E	274	CYS	2.7
1	E	75	THR	2.7
1	B	478	ASP	2.6
1	C	483	PHE	2.6
1	D	292	SER	2.5
1	F	45	LEU	2.5
1	B	77	GLU	2.5
1	A	219	GLN	2.5
1	A	37	LYS	2.5
1	E	213	SER	2.4
1	B	79	GLY	2.4
1	E	294	GLN	2.4
1	A	454	ILE	2.3
1	D	295	GLN	2.3
1	E	276	PRO	2.3
1	D	483	PHE	2.3
1	E	449	ASN	2.3
1	C	450	SER	2.2
1	E	278	ILE	2.2
1	E	296	VAL	2.2
1	D	449	ASN	2.2
1	E	201	ILE	2.2
1	C	76	VAL	2.2
1	C	482	ARG	2.2
1	B	215	VAL	2.2
1	E	480	ARG	2.2
1	C	213	SER	2.2
1	A	148	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	148	GLN	2.1
1	E	291	ASP	2.1
1	F	450	SER	2.1
1	E	292	SER	2.1
1	A	294	GLN	2.1
1	B	451	ALA	2.0
1	C	14	PRO	2.0
1	E	187	TYR	2.0
1	C	77	GLU	2.0
1	E	217	GLY	2.0
1	B	483	PHE	2.0
1	D	288	VAL	2.0
1	B	34	LEU	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 monosaccharides 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.