



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:15 AM UTC

PDB ID : 1OY0 / pdb_00001oy0
Title : The crystal Structure of the First Enzyme of Pantothenate Biosynthetic Pathway, Ketopantoate Hydroxymethyltransferase from Mycobacterium Tuberculosis Shows a Decameric Assembly and Terminal Helix-Swapping
Authors : Chaudhuri, B.N.; Sawaya, M.R.; Kim, C.Y.; Waldo, G.S.; Park, M.S.; Terwilliger, T.C.; Yeates, T.O.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-04-03
Resolution : 2.80 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

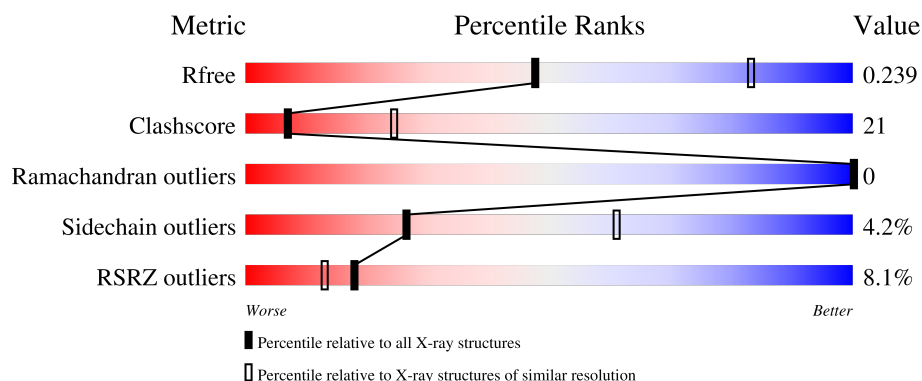
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	281	5% 58% 28% • 12%
1	B	281	8% 58% 29% • 12%
1	C	281	9% 56% 30% • 12%
1	D	281	6% 57% 30% • 12%
1	E	281	8% 57% 30% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9245 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 Ketopantoate hydroxymethyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1827	1160	319	340	8			
1	B	248	Total	C	N	O	S	0	0	0
			1827	1160	319	340	8			
1	C	248	Total	C	N	O	S	0	0	0
			1827	1160	319	340	8			
1	D	248	Total	C	N	O	S	0	0	0
			1827	1160	319	340	8			
1	E	248	Total	C	N	O	S	0	0	0
			1827	1160	319	340	8			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total	O	0	0
			28	28		
3	B	18	Total	O	0	0
			18	18		

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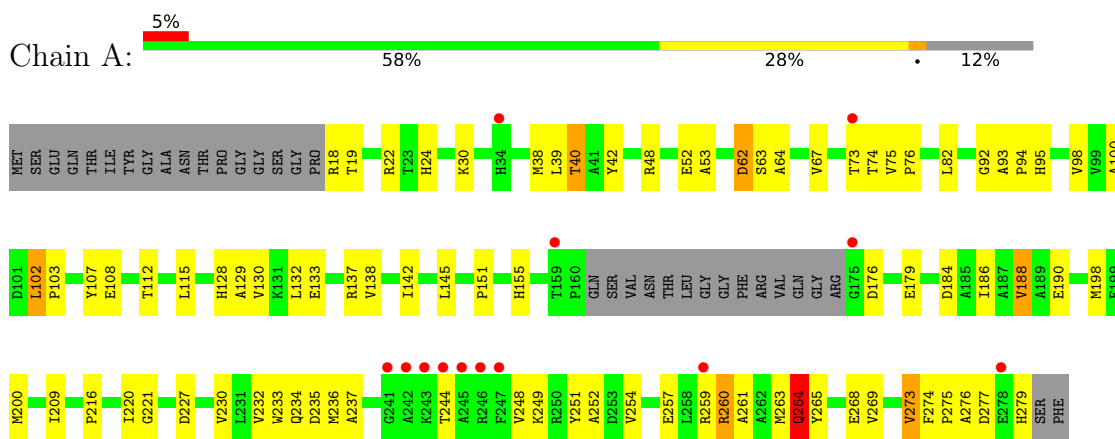
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	19	Total	O	0	0
			19	19		
3	D	20	Total	O	0	0
			20	20		
3	E	20	Total	O	0	0
			20	20		

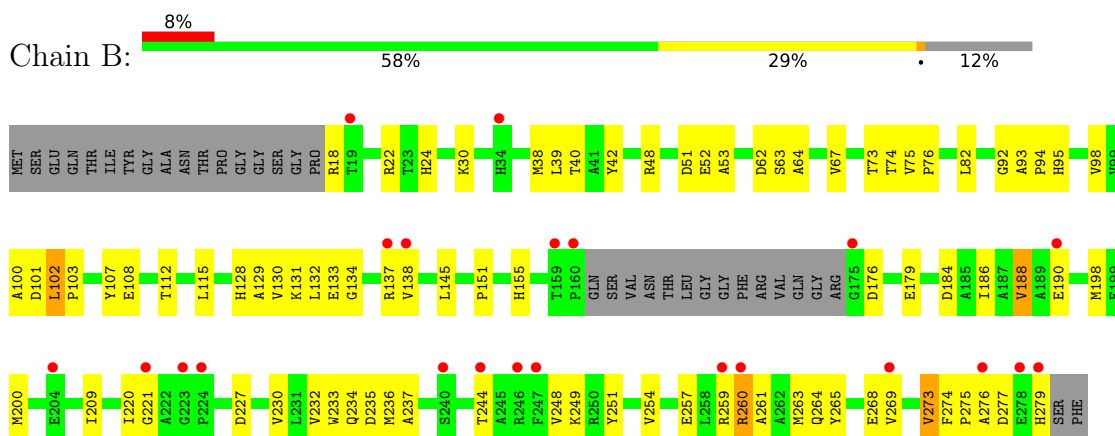
3 Residue-property plots [i](#)

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.

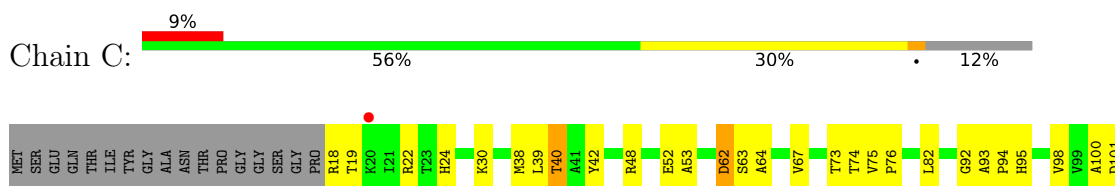
- Molecule 1: Ketopantoate hydroxymethyltransferase

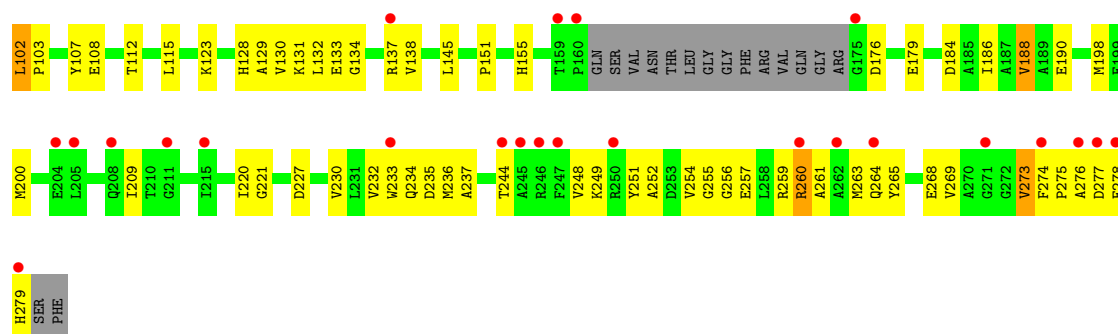


- Molecule 1: Ketopantoate hydroxymethyltransferase

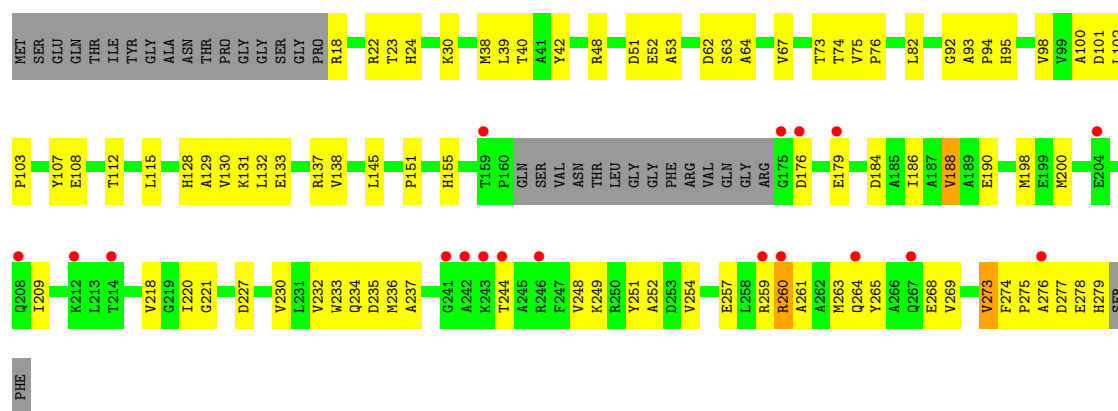


- Molecule 1: Ketopantoate hydroxymethyltransferase

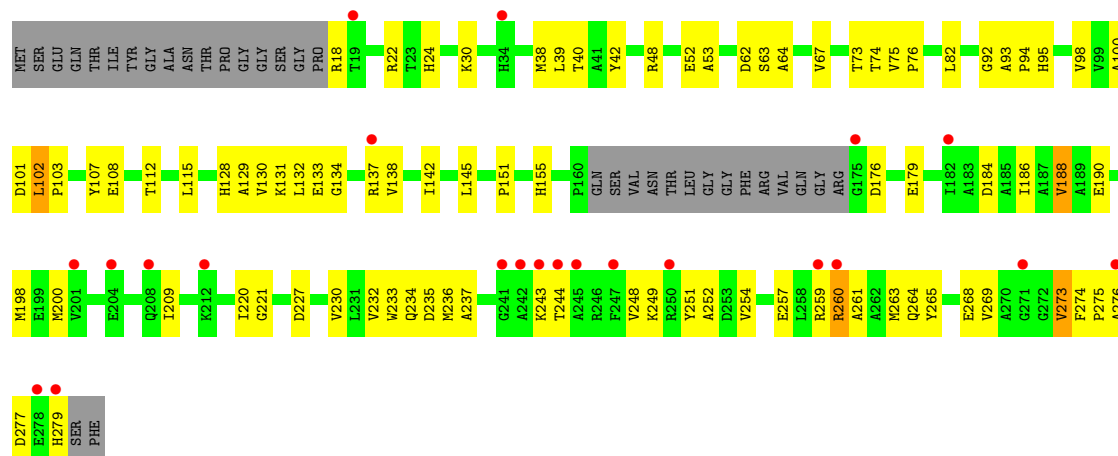




• Molecule 1: Ketopantoate hydroxymethyltransferase



• Molecule 1: Ketopantoate hydroxymethyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.80Å 106.80Å 224.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	92.53 – 2.80 92.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (92.53-2.80) 97.8 (92.49-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.82Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.275 0.240 , 0.239	Depositor DCC
R_{free} test set	1822 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9245	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.47	0/1865	1.01	9/2539 (0.4%)
1	B	0.44	0/1865	0.97	7/2539 (0.3%)
1	C	0.44	0/1865	0.95	8/2539 (0.3%)
1	D	0.46	0/1865	0.95	6/2539 (0.2%)
1	E	0.45	0/1865	0.96	7/2539 (0.3%)
All	All	0.45	0/9325	0.97	37/12695 (0.3%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	GLN	OE1-CD-NE2	-10.25	112.35	122.60
1	A	62	ASP	N-CA-C	-8.88	102.15	113.16
1	B	63	SER	N-CA-C	-8.05	103.44	113.18
1	A	63	SER	N-CA-C	-7.56	103.94	113.01
1	A	264	GLN	CG-CD-NE2	6.73	126.49	116.40
1	C	62	ASP	N-CA-C	-6.39	105.47	113.20
1	D	62	ASP	N-CA-C	-6.28	105.60	113.20
1	C	63	SER	N-CA-C	-6.10	105.55	112.87
1	E	63	SER	N-CA-C	-5.83	106.02	113.01
1	B	62	ASP	N-CA-C	-5.81	106.05	113.02
1	E	62	ASP	N-CA-C	-5.75	106.25	113.20
1	E	102	LEU	CA-C-N	5.65	125.60	119.78
1	E	102	LEU	C-N-CA	5.65	125.60	119.78
1	C	102	LEU	CA-C-N	5.63	125.58	119.78
1	C	102	LEU	C-N-CA	5.63	125.58	119.78
1	B	53	ALA	N-CA-C	-5.62	105.77	113.30
1	A	102	LEU	CA-C-N	5.61	125.56	119.78
1	A	102	LEU	C-N-CA	5.61	125.56	119.78
1	B	102	LEU	CA-C-N	5.52	125.83	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	LEU	C-N-CA	5.52	125.83	119.92
1	C	53	ALA	N-CA-C	-5.46	105.98	113.30
1	A	53	ALA	N-CA-C	-5.36	106.11	113.30
1	D	63	SER	N-CA-C	-5.36	106.58	113.01
1	E	53	ALA	N-CA-C	-5.35	106.13	113.30
1	A	93	ALA	CA-C-N	5.33	125.00	119.56
1	A	93	ALA	C-N-CA	5.33	125.00	119.56
1	C	93	ALA	CA-C-N	5.29	124.96	119.56
1	C	93	ALA	C-N-CA	5.29	124.96	119.56
1	D	53	ALA	N-CA-C	-5.26	106.25	113.30
1	C	278	GLU	N-CA-C	-5.22	106.60	112.87
1	B	93	ALA	CA-C-N	5.17	124.83	119.56
1	B	93	ALA	C-N-CA	5.17	124.83	119.56
1	D	93	ALA	CA-C-N	5.07	124.74	119.56
1	D	93	ALA	C-N-CA	5.07	124.74	119.56
1	E	93	ALA	CA-C-N	5.04	124.70	119.56
1	E	93	ALA	C-N-CA	5.04	124.70	119.56
1	D	278	GLU	N-CA-C	-5.04	106.83	112.87

There are no chirality outliers.

There are no planarity outliers.

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	1827	0	1814	82	0
1	B	1827	0	1814	73	0
1	C	1827	0	1814	78	0
1	D	1827	0	1814	75	0
1	E	1827	0	1814	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	28	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	19	0	0	1	0
3	D	20	0	0	1	0
3	E	20	0	0	0	0
All	All	9245	0	9070	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (384) 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:73:THR:HG22	1:C:75:VAL:H	1.15	1.11
1:E:200:MET:HE2	1:E:200:MET:HA	1.34	1.09
1:D:73:THR:HG22	1:D:75:VAL:H	1.12	1.09
1:A:73:THR:HG22	1:A:75:VAL:H	1.15	1.07
1:B:73:THR:HG22	1:B:75:VAL:H	1.18	1.07
1:E:73:THR:HG22	1:E:75:VAL:H	1.19	1.04
1:E:67:VAL:HG11	1:E:234:GLN:HG3	1.42	1.00
1:B:67:VAL:HG11	1:B:234:GLN:HG3	1.43	1.00
1:D:67:VAL:HG11	1:D:234:GLN:HG3	1.40	1.00
1:A:67:VAL:HG11	1:A:234:GLN:HG3	1.41	1.00
1:A:40:THR:HG22	1:A:233:TRP:H	1.26	1.00
1:C:40:THR:HG22	1:C:233:TRP:H	1.27	0.99
1:C:67:VAL:HG11	1:C:234:GLN:HG3	1.43	0.98
1:D:40:THR:HG22	1:D:233:TRP:H	1.27	0.98
1:E:40:THR:HG22	1:E:233:TRP:H	1.25	0.97
1:E:98:VAL:H	1:E:128:HIS:HD2	1.11	0.97
1:B:40:THR:HG22	1:B:233:TRP:H	1.28	0.96
1:A:98:VAL:H	1:A:128:HIS:HD2	1.13	0.96
1:C:98:VAL:H	1:C:128:HIS:HD2	1.13	0.96
1:B:98:VAL:H	1:B:128:HIS:HD2	1.13	0.91
1:E:276:ALA:H	1:E:279:HIS:HD2	1.17	0.91
1:B:276:ALA:H	1:B:279:HIS:HD2	1.17	0.91
1:D:276:ALA:H	1:D:279:HIS:HD2	1.19	0.90
1:D:98:VAL:H	1:D:128:HIS:HD2	1.12	0.90
1:C:276:ALA:H	1:C:279:HIS:HD2	1.18	0.89
1:A:276:ALA:H	1:A:279:HIS:HD2	1.17	0.87
1:D:98:VAL:H	1:D:128:HIS:CD2	1.92	0.87
1:E:98:VAL:H	1:E:128:HIS:CD2	1.92	0.86
1:A:98:VAL:H	1:A:128:HIS:CD2	1.92	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD12	1:A:132:LEU:HD13	1.58	0.86
1:C:98:VAL:H	1:C:128:HIS:CD2	1.93	0.86
1:B:98:VAL:H	1:B:128:HIS:CD2	1.94	0.86
1:D:102:LEU:HD12	1:D:132:LEU:HD13	1.59	0.85
1:B:102:LEU:HD12	1:B:132:LEU:HD13	1.60	0.83
1:B:268:GLU:HB3	1:B:273:VAL:HG22	1.61	0.82
1:E:268:GLU:HB3	1:E:273:VAL:HG22	1.60	0.82
1:E:102:LEU:HD12	1:E:132:LEU:HD13	1.62	0.82
1:A:73:THR:HG22	1:A:75:VAL:N	1.95	0.80
1:D:38:MET:HE2	1:D:218:VAL:HG11	1.63	0.80
1:D:268:GLU:HB3	1:D:273:VAL:HG22	1.62	0.80
1:A:268:GLU:HB3	1:A:273:VAL:HG22	1.63	0.80
1:C:102:LEU:HD12	1:C:132:LEU:HD13	1.63	0.80
1:E:73:THR:HG22	1:E:75:VAL:N	1.95	0.80
1:C:73:THR:HG22	1:C:75:VAL:N	1.96	0.80
1:C:268:GLU:HB3	1:C:273:VAL:HG22	1.62	0.80
1:D:73:THR:HG22	1:D:75:VAL:N	1.95	0.78
1:B:73:THR:HG22	1:B:75:VAL:N	1.97	0.78
1:E:200:MET:HE2	1:E:200:MET:CA	2.14	0.76
1:C:82:LEU:HD12	1:C:103:PRO:HG3	1.68	0.75
1:D:82:LEU:HD12	1:D:103:PRO:HG3	1.70	0.74
1:E:82:LEU:HD12	1:E:103:PRO:HG3	1.68	0.74
1:E:101:ASP:OD1	1:E:131:LYS:HE2	1.89	0.72
1:E:73:THR:HG22	1:E:74:THR:N	2.05	0.72
1:A:82:LEU:HD12	1:A:103:PRO:HG3	1.71	0.72
1:C:18:ARG:HG2	1:C:95:HIS:CD2	2.25	0.72
1:A:73:THR:HG22	1:A:74:THR:N	2.06	0.71
1:B:82:LEU:HD12	1:B:103:PRO:HG3	1.71	0.71
1:A:102:LEU:HD12	1:A:132:LEU:CD1	2.21	0.70
1:D:98:VAL:N	1:D:128:HIS:HD2	1.89	0.70
1:C:73:THR:HG22	1:C:74:THR:N	2.06	0.70
1:A:98:VAL:N	1:A:128:HIS:HD2	1.90	0.69
1:A:67:VAL:CG1	1:A:234:GLN:HG3	2.21	0.69
1:E:200:MET:HA	1:E:200:MET:CE	2.19	0.69
1:A:73:THR:CG2	1:A:74:THR:N	2.56	0.69
1:B:67:VAL:CG1	1:B:234:GLN:HG3	2.22	0.69
1:E:73:THR:CG2	1:E:74:THR:N	2.56	0.69
1:C:98:VAL:N	1:C:128:HIS:HD2	1.91	0.68
1:D:102:LEU:HD12	1:D:132:LEU:CD1	2.23	0.68
1:B:100:ALA:O	1:B:130:VAL:HA	1.93	0.67
1:E:98:VAL:N	1:E:128:HIS:HD2	1.89	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD12	1:B:132:LEU:CD1	2.24	0.67
1:C:73:THR:CG2	1:C:74:THR:N	2.58	0.67
1:B:98:VAL:N	1:B:128:HIS:HD2	1.91	0.67
1:B:73:THR:HG22	1:B:74:THR:N	2.08	0.66
1:D:73:THR:HG22	1:D:74:THR:N	2.08	0.66
1:D:73:THR:CG2	1:D:74:THR:N	2.58	0.66
1:A:48:ARG:O	1:A:52:GLU:HG2	1.95	0.66
1:E:67:VAL:CG1	1:E:234:GLN:HG3	2.22	0.66
1:E:274:PHE:CD1	1:E:275:PRO:HA	2.31	0.66
1:D:274:PHE:CD1	1:D:275:PRO:HA	2.31	0.65
1:E:102:LEU:HD12	1:E:132:LEU:CD1	2.25	0.65
1:A:75:VAL:O	1:C:123:LYS:HG2	1.97	0.65
1:B:73:THR:CG2	1:B:74:THR:N	2.59	0.65
1:C:40:THR:HG22	1:C:233:TRP:N	2.08	0.65
1:D:38:MET:HE3	1:D:230:VAL:HG21	1.77	0.65
1:D:67:VAL:CG1	1:D:234:GLN:HG3	2.20	0.65
1:A:274:PHE:CD1	1:A:275:PRO:HA	2.31	0.65
1:C:67:VAL:CG1	1:C:234:GLN:HG3	2.22	0.65
1:C:274:PHE:CD1	1:C:275:PRO:HA	2.31	0.65
1:D:101:ASP:OD1	1:D:131:LYS:HE2	1.96	0.65
1:A:40:THR:HG22	1:A:233:TRP:N	2.07	0.65
1:B:274:PHE:CD1	1:B:275:PRO:HA	2.31	0.65
1:C:102:LEU:HD12	1:C:132:LEU:CD1	2.26	0.64
1:E:48:ARG:O	1:E:52:GLU:HG2	1.97	0.64
1:A:107:TYR:CG	1:A:132:LEU:HD11	2.33	0.64
1:B:48:ARG:O	1:B:52:GLU:HG2	1.97	0.64
1:D:18:ARG:HG2	1:D:95:HIS:CD2	2.33	0.63
1:B:176:ASP:HA	1:B:179:GLU:OE2	1.99	0.63
1:C:48:ARG:O	1:C:52:GLU:HG2	1.99	0.62
1:D:48:ARG:O	1:D:52:GLU:HG2	1.99	0.62
1:B:30:LYS:HG3	1:B:227:ASP:OD1	2.00	0.62
1:B:18:ARG:NH2	1:B:51:ASP:O	2.33	0.61
1:C:107:TYR:CG	1:C:132:LEU:HD11	2.34	0.61
1:B:138:VAL:HG12	1:B:138:VAL:O	2.00	0.61
1:D:40:THR:HG22	1:D:233:TRP:N	2.08	0.61
1:C:137:ARG:HG3	1:C:138:VAL:HG23	1.83	0.61
1:D:107:TYR:CG	1:D:132:LEU:HD11	2.36	0.61
1:E:107:TYR:CG	1:E:132:LEU:HD11	2.35	0.61
1:B:107:TYR:CG	1:B:132:LEU:HD11	2.36	0.61
1:C:30:LYS:HG3	1:C:227:ASP:OD1	2.01	0.60
1:B:137:ARG:HG3	1:B:138:VAL:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:O	1:D:138:VAL:HG12	2.01	0.60
1:A:137:ARG:HG3	1:A:138:VAL:HG23	1.82	0.60
1:C:138:VAL:HG12	1:C:138:VAL:O	2.00	0.60
1:D:30:LYS:HG3	1:D:227:ASP:OD1	2.02	0.60
1:C:30:LYS:HA	3:C:908:HOH:O	2.01	0.60
1:D:137:ARG:HG3	1:D:138:VAL:HG23	1.82	0.60
1:B:40:THR:HG22	1:B:233:TRP:N	2.09	0.60
1:E:40:THR:HG22	1:E:233:TRP:N	2.07	0.60
1:A:30:LYS:HG3	1:A:227:ASP:OD1	2.02	0.60
1:A:138:VAL:HG12	1:A:138:VAL:O	2.01	0.59
1:E:82:LEU:CD1	1:E:103:PRO:HG3	2.31	0.59
1:C:176:ASP:HA	1:C:179:GLU:OE2	2.01	0.59
1:A:100:ALA:O	1:A:130:VAL:HA	2.03	0.59
1:E:73:THR:CG2	1:E:74:THR:H	2.15	0.59
1:E:220:ILE:HG23	1:E:220:ILE:O	2.03	0.59
1:C:100:ALA:O	1:C:130:VAL:HA	2.02	0.59
1:E:176:ASP:HA	1:E:179:GLU:OE2	2.03	0.58
1:A:220:ILE:HG23	1:A:220:ILE:O	2.03	0.58
1:E:30:LYS:HG3	1:E:227:ASP:OD1	2.04	0.58
1:B:276:ALA:H	1:B:279:HIS:CD2	2.10	0.58
1:A:176:ASP:HA	1:A:179:GLU:OE2	2.04	0.57
1:C:82:LEU:CD1	1:C:103:PRO:HG3	2.32	0.57
1:E:73:THR:CG2	1:E:75:VAL:HG23	2.34	0.57
1:E:200:MET:CE	1:E:221:GLY:HA3	2.34	0.57
1:A:82:LEU:CD1	1:A:103:PRO:HG3	2.34	0.57
1:E:137:ARG:HG3	1:E:138:VAL:HG23	1.84	0.57
1:B:220:ILE:HG23	1:B:220:ILE:O	2.04	0.57
1:E:138:VAL:HG12	1:E:138:VAL:O	2.03	0.57
1:A:18:ARG:HG2	1:A:95:HIS:CD2	2.40	0.57
1:A:73:THR:CG2	1:A:74:THR:H	2.17	0.57
1:E:133:GLU:HA	1:E:155:HIS:HB3	1.87	0.57
1:E:265:TYR:O	1:E:269:VAL:HG23	2.05	0.57
1:E:276:ALA:H	1:E:279:HIS:CD2	2.09	0.57
1:D:133:GLU:HA	1:D:155:HIS:HB3	1.87	0.57
1:D:100:ALA:O	1:D:130:VAL:HA	2.05	0.57
1:D:115:LEU:HA	1:D:145:LEU:CD2	2.35	0.57
1:D:73:THR:CG2	1:D:75:VAL:HG23	2.35	0.57
1:B:18:ARG:HG2	1:B:95:HIS:CD2	2.40	0.56
1:E:75:VAL:N	1:E:76:PRO:HD2	2.20	0.56
1:B:115:LEU:HA	1:B:145:LEU:CD2	2.35	0.56
1:C:115:LEU:HA	1:C:145:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:MET:HE1	1:D:209:ILE:HD12	1.88	0.56
1:A:198:MET:HE1	1:A:209:ILE:HD12	1.85	0.56
1:D:82:LEU:CD1	1:D:103:PRO:HG3	2.35	0.56
1:D:220:ILE:O	1:D:220:ILE:HG23	2.06	0.56
1:C:265:TYR:O	1:C:269:VAL:HG23	2.04	0.56
1:A:133:GLU:HA	1:A:155:HIS:HB3	1.87	0.56
1:A:265:TYR:O	1:A:269:VAL:HG23	2.06	0.56
1:C:198:MET:HE1	1:C:209:ILE:HD12	1.88	0.56
1:E:100:ALA:O	1:E:130:VAL:HA	2.06	0.55
1:C:220:ILE:HG23	1:C:220:ILE:O	2.04	0.55
1:C:276:ALA:H	1:C:279:HIS:CD2	2.10	0.55
1:C:256:GLY:HA2	1:C:259:ARG:HD3	1.88	0.55
1:E:115:LEU:HA	1:E:145:LEU:CD2	2.36	0.55
1:A:115:LEU:HA	1:A:145:LEU:CD2	2.35	0.55
1:B:82:LEU:CD1	1:B:103:PRO:HG3	2.34	0.55
1:A:198:MET:CE	1:A:209:ILE:HD12	2.37	0.55
1:B:232:VAL:HG12	1:B:234:GLN:HG2	1.89	0.55
1:C:200:MET:CE	1:C:221:GLY:HA3	2.37	0.55
1:B:265:TYR:O	1:B:269:VAL:HG23	2.06	0.54
1:C:73:THR:CG2	1:C:74:THR:H	2.20	0.54
1:E:232:VAL:HG12	1:E:234:GLN:HG2	1.88	0.54
1:C:133:GLU:HA	1:C:155:HIS:HB3	1.88	0.54
1:B:73:THR:CG2	1:B:75:VAL:HG23	2.37	0.54
1:A:200:MET:CE	1:A:221:GLY:HA3	2.37	0.54
1:A:276:ALA:H	1:A:279:HIS:CD2	2.09	0.54
1:C:39:LEU:HD21	1:C:236:MET:HE2	1.89	0.54
1:A:39:LEU:HD21	1:A:236:MET:HE2	1.90	0.54
1:B:75:VAL:N	1:B:76:PRO:HD2	2.23	0.54
1:C:73:THR:CG2	1:C:75:VAL:HG23	2.37	0.54
1:D:200:MET:CE	1:D:221:GLY:HA3	2.38	0.54
1:C:232:VAL:HG12	1:C:234:GLN:HG2	1.88	0.53
1:B:259:ARG:O	1:B:263:MET:HG3	2.09	0.53
1:D:232:VAL:HG12	1:D:234:GLN:HG2	1.89	0.53
1:E:198:MET:HE1	1:E:209:ILE:HD12	1.90	0.53
1:B:39:LEU:HD21	1:B:236:MET:HE2	1.90	0.53
1:D:276:ALA:H	1:D:279:HIS:CD2	2.11	0.53
1:A:232:VAL:HG12	1:A:234:GLN:HG2	1.90	0.53
1:A:75:VAL:N	1:A:76:PRO:HD2	2.24	0.53
1:D:259:ARG:O	1:D:263:MET:HG3	2.09	0.53
1:B:133:GLU:HA	1:B:155:HIS:HB3	1.90	0.52
1:A:259:ARG:O	1:A:263:MET:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:TYR:HE2	1:B:234:GLN:HE21	1.58	0.52
1:B:198:MET:HE1	1:B:209:ILE:HD12	1.90	0.52
1:B:200:MET:CE	1:B:221:GLY:HA3	2.40	0.52
1:D:75:VAL:N	1:D:76:PRO:HD2	2.24	0.52
1:D:38:MET:HE3	1:D:230:VAL:CG2	2.40	0.52
1:A:73:THR:CG2	1:A:75:VAL:HG23	2.40	0.52
1:E:39:LEU:HD21	1:E:236:MET:HE2	1.92	0.52
1:D:176:ASP:HA	1:D:179:GLU:OE2	2.09	0.52
1:B:235:ASP:HB3	1:B:248:VAL:HG11	1.92	0.51
1:C:235:ASP:HB3	1:C:248:VAL:HG11	1.92	0.51
1:D:42:TYR:HE2	1:D:234:GLN:HE21	1.56	0.51
1:E:200:MET:HE1	1:E:221:GLY:HA3	1.91	0.51
1:A:42:TYR:HE2	1:A:234:GLN:HE21	1.59	0.51
1:C:75:VAL:N	1:C:76:PRO:HD2	2.25	0.51
1:D:198:MET:CE	1:D:209:ILE:HD12	2.41	0.51
1:E:259:ARG:O	1:E:263:MET:HG3	2.11	0.51
1:C:259:ARG:O	1:C:263:MET:HG3	2.10	0.51
1:D:277:ASP:C	1:D:279:HIS:N	2.67	0.51
1:C:277:ASP:C	1:C:279:HIS:N	2.69	0.51
1:C:255:GLY:O	1:C:259:ARG:HG3	2.11	0.51
1:D:38:MET:HE2	1:D:230:VAL:HB	1.93	0.51
1:D:265:TYR:O	1:D:269:VAL:HG23	2.11	0.51
1:E:42:TYR:HE2	1:E:234:GLN:HE21	1.59	0.51
1:E:235:ASP:HB3	1:E:248:VAL:HG11	1.92	0.51
1:A:235:ASP:HB3	1:A:248:VAL:HG11	1.93	0.50
1:D:39:LEU:HD21	1:D:236:MET:HE2	1.92	0.50
1:C:38:MET:HE3	1:C:230:VAL:HG21	1.92	0.50
1:D:73:THR:CG2	1:D:74:THR:H	2.23	0.50
1:B:38:MET:HE3	1:B:230:VAL:HG21	1.93	0.50
1:B:73:THR:CG2	1:B:74:THR:H	2.23	0.50
1:A:277:ASP:C	1:A:279:HIS:H	2.19	0.50
1:D:73:THR:HG21	1:D:75:VAL:HG23	1.94	0.50
1:A:40:THR:CG2	1:A:232:VAL:HA	2.42	0.50
1:E:101:ASP:CG	1:E:131:LYS:HE2	2.37	0.49
1:B:237:ALA:HB1	1:B:254:VAL:CG2	2.43	0.49
1:E:277:ASP:C	1:E:279:HIS:N	2.70	0.49
1:E:38:MET:HE3	1:E:230:VAL:HG21	1.95	0.49
1:B:249:LYS:HD3	1:B:251:TYR:CZ	2.47	0.49
1:D:108:GLU:OE1	1:D:108:GLU:N	2.45	0.49
1:C:42:TYR:HE2	1:C:234:GLN:HE21	1.60	0.49
1:C:198:MET:CE	1:C:209:ILE:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ASP:C	1:A:279:HIS:N	2.68	0.49
1:E:42:TYR:CD1	1:E:64:ALA:HB2	2.47	0.49
1:E:108:GLU:OE1	1:E:108:GLU:N	2.43	0.49
1:A:38:MET:HE3	1:A:230:VAL:HG21	1.95	0.48
1:C:48:ARG:HA	1:C:92:GLY:O	2.13	0.48
1:D:249:LYS:HD3	1:D:251:TYR:CZ	2.48	0.48
1:D:277:ASP:C	1:D:279:HIS:H	2.19	0.48
1:A:249:LYS:HD3	1:A:251:TYR:CZ	2.48	0.48
1:C:200:MET:HE1	1:C:221:GLY:HA3	1.95	0.48
1:E:237:ALA:HB1	1:E:254:VAL:CG2	2.43	0.48
1:B:73:THR:HG21	1:B:75:VAL:HG23	1.96	0.48
1:B:277:ASP:C	1:B:279:HIS:H	2.19	0.48
1:D:235:ASP:HB3	1:D:248:VAL:HG11	1.95	0.48
1:A:115:LEU:HA	1:A:145:LEU:HD21	1.95	0.48
1:E:249:LYS:HD3	1:E:251:TYR:CZ	2.49	0.48
1:D:198:MET:HE1	1:D:209:ILE:HB	1.96	0.48
1:D:42:TYR:CD1	1:D:64:ALA:HB2	2.48	0.48
1:C:40:THR:HG21	1:C:232:VAL:HG13	1.96	0.48
1:D:40:THR:CG2	1:D:232:VAL:HA	2.43	0.48
1:C:108:GLU:N	1:C:108:GLU:OE1	2.45	0.48
1:E:277:ASP:C	1:E:279:HIS:H	2.22	0.48
1:E:73:THR:HG21	1:E:75:VAL:HG23	1.95	0.47
1:E:198:MET:CE	1:E:209:ILE:HD12	2.44	0.47
1:C:220:ILE:HD12	1:C:230:VAL:O	2.14	0.47
1:C:277:ASP:C	1:C:279:HIS:H	2.21	0.47
1:D:115:LEU:HA	1:D:145:LEU:HD21	1.97	0.47
1:D:200:MET:HE2	1:D:200:MET:HA	1.96	0.47
1:D:220:ILE:HD12	1:D:230:VAL:O	2.14	0.47
1:A:108:GLU:OE1	1:A:108:GLU:N	2.45	0.47
1:C:186:ILE:O	1:C:190:GLU:HG2	2.14	0.47
1:C:249:LYS:HD3	1:C:251:TYR:CZ	2.49	0.47
1:A:62:ASP:C	1:A:64:ALA:N	2.73	0.47
1:B:40:THR:HG21	1:B:232:VAL:HG13	1.97	0.47
1:B:277:ASP:C	1:B:279:HIS:N	2.68	0.47
1:D:101:ASP:CG	1:D:131:LYS:HE2	2.40	0.47
1:E:115:LEU:HA	1:E:145:LEU:HD21	1.96	0.47
1:C:40:THR:CG2	1:C:232:VAL:HA	2.44	0.47
1:C:73:THR:HG21	1:C:75:VAL:HG23	1.96	0.47
1:A:18:ARG:HG3	1:A:19:THR:H	1.80	0.47
1:A:42:TYR:CD1	1:A:64:ALA:HB2	2.50	0.47
1:B:200:MET:HA	1:B:200:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ASP:O	1:D:188:VAL:HB	2.15	0.46
1:A:186:ILE:O	1:A:190:GLU:HG2	2.15	0.46
1:B:42:TYR:CD1	1:B:64:ALA:HB2	2.49	0.46
1:C:42:TYR:CD1	1:C:64:ALA:HB2	2.49	0.46
1:C:237:ALA:HB1	1:C:254:VAL:CG2	2.44	0.46
1:E:40:THR:CG2	1:E:232:VAL:HA	2.45	0.46
1:A:129:ALA:HB2	1:A:151:PRO:HB2	1.98	0.46
1:B:22:ARG:HB2	1:B:24:HIS:CE1	2.51	0.46
1:E:102:LEU:HA	1:E:103:PRO:HD3	1.79	0.46
1:E:220:ILE:HD12	1:E:230:VAL:O	2.15	0.46
1:B:198:MET:CE	1:B:209:ILE:HD12	2.45	0.46
1:B:115:LEU:HA	1:B:145:LEU:HD21	1.97	0.46
1:C:200:MET:HE2	1:C:200:MET:HA	1.97	0.46
1:D:40:THR:HG21	1:D:232:VAL:HG13	1.97	0.46
1:A:216:PRO:HB3	3:A:906:HOH:O	2.16	0.46
1:B:40:THR:CG2	1:B:232:VAL:HA	2.46	0.46
1:C:22:ARG:HB2	1:C:24:HIS:CE1	2.51	0.45
1:C:62:ASP:C	1:C:64:ALA:N	2.72	0.45
1:D:23:THR:HG23	3:D:911:HOH:O	2.16	0.45
1:A:200:MET:HE2	1:A:200:MET:HA	1.97	0.45
1:C:115:LEU:HA	1:C:145:LEU:HD21	1.97	0.45
1:E:200:MET:CA	1:E:200:MET:CE	2.87	0.45
1:A:184:ASP:O	1:A:188:VAL:HB	2.17	0.45
1:B:108:GLU:OE1	1:B:108:GLU:N	2.47	0.45
1:B:260:ARG:O	1:B:261:ALA:C	2.58	0.45
1:C:184:ASP:O	1:C:188:VAL:HB	2.17	0.45
1:E:75:VAL:N	1:E:76:PRO:CD	2.80	0.45
1:A:18:ARG:HG3	1:A:19:THR:N	2.31	0.45
1:A:48:ARG:HA	1:A:92:GLY:O	2.17	0.45
1:A:73:THR:HG23	1:A:74:THR:H	1.82	0.45
1:D:200:MET:HE1	1:D:221:GLY:HA3	1.98	0.45
1:E:129:ALA:HB2	1:E:151:PRO:HB2	1.98	0.45
1:A:62:ASP:OD1	1:A:62:ASP:N	2.45	0.45
1:A:264:GLN:NE2	1:A:268:GLU:OE1	2.50	0.45
1:B:48:ARG:HA	1:B:92:GLY:O	2.16	0.45
1:B:220:ILE:HD12	1:B:230:VAL:O	2.17	0.45
1:A:102:LEU:HA	1:A:103:PRO:HD3	1.76	0.45
1:A:220:ILE:HD12	1:A:230:VAL:O	2.16	0.45
1:E:40:THR:HG21	1:E:232:VAL:HG13	1.99	0.45
1:A:73:THR:HG21	1:A:75:VAL:HG23	1.99	0.45
1:D:48:ARG:HA	1:D:92:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ARG:HA	1:E:92:GLY:O	2.17	0.44
1:E:260:ARG:O	1:E:261:ALA:C	2.60	0.44
1:A:22:ARG:HB2	1:A:24:HIS:CE1	2.51	0.44
1:A:40:THR:HG21	1:A:232:VAL:HG13	1.99	0.44
1:D:237:ALA:HB1	1:D:254:VAL:CG2	2.47	0.44
1:B:129:ALA:HB2	1:B:151:PRO:HB2	2.00	0.44
1:C:260:ARG:O	1:C:261:ALA:C	2.59	0.44
1:E:22:ARG:HB2	1:E:24:HIS:CE1	2.52	0.44
1:E:186:ILE:O	1:E:190:GLU:HG2	2.18	0.44
1:A:198:MET:HE1	1:A:209:ILE:HB	2.00	0.44
1:D:129:ALA:HB2	1:D:151:PRO:HB2	2.00	0.44
1:A:227:ASP:HB3	3:A:906:HOH:O	2.18	0.44
1:A:237:ALA:HB1	1:A:254:VAL:CG2	2.47	0.44
1:B:48:ARG:HH12	1:B:94:PRO:HD3	1.83	0.44
1:B:200:MET:HE1	1:B:221:GLY:HA3	2.00	0.44
1:A:260:ARG:O	1:A:261:ALA:C	2.60	0.44
1:B:101:ASP:OD1	1:B:131:LYS:HE2	2.17	0.44
1:A:18:ARG:CG	1:A:19:THR:N	2.80	0.43
1:A:251:TYR:O	1:A:252:ALA:HB2	2.18	0.43
1:E:184:ASP:O	1:E:188:VAL:HB	2.17	0.43
1:B:186:ILE:O	1:B:190:GLU:HG2	2.17	0.43
1:D:260:ARG:O	1:D:261:ALA:C	2.61	0.43
1:E:18:ARG:HG2	1:E:95:HIS:CD2	2.52	0.43
1:E:73:THR:HG23	1:E:74:THR:H	1.83	0.43
1:B:184:ASP:O	1:B:188:VAL:HB	2.18	0.43
1:C:129:ALA:HB2	1:C:151:PRO:HB2	2.01	0.43
1:D:22:ARG:HB2	1:D:24:HIS:CE1	2.53	0.43
1:A:200:MET:HE1	1:A:221:GLY:HA3	2.00	0.43
1:D:186:ILE:O	1:D:190:GLU:HG2	2.18	0.43
1:D:48:ARG:HH12	1:D:94:PRO:HD3	1.84	0.43
1:B:102:LEU:HA	1:B:103:PRO:HD3	1.79	0.43
1:C:18:ARG:HG3	1:C:19:THR:N	2.34	0.43
1:E:251:TYR:O	1:E:252:ALA:HB2	2.20	0.42
1:C:101:ASP:OD1	1:C:131:LYS:HE2	2.20	0.42
1:C:48:ARG:HH12	1:C:94:PRO:HD3	1.84	0.42
1:E:48:ARG:HH12	1:E:94:PRO:HD3	1.84	0.42
1:B:134:GLY:HA3	1:B:138:VAL:HG21	2.02	0.42
1:A:75:VAL:N	1:A:76:PRO:CD	2.83	0.42
1:C:251:TYR:O	1:C:252:ALA:HB2	2.20	0.42
1:A:48:ARG:HH12	1:A:94:PRO:HD3	1.85	0.42
1:C:134:GLY:HA3	1:C:138:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:MET:HE2	1:C:230:VAL:HB	2.03	0.41
1:A:220:ILE:HB	1:A:230:VAL:HG13	2.02	0.41
1:A:232:VAL:CG1	1:A:234:GLN:HG2	2.50	0.41
1:E:134:GLY:HA3	1:E:138:VAL:HG21	2.02	0.41
1:B:75:VAL:N	1:B:76:PRO:CD	2.83	0.41
1:B:220:ILE:HB	1:B:230:VAL:HG13	2.02	0.41
1:D:18:ARG:NH2	1:D:51:ASP:O	2.42	0.41
1:C:220:ILE:HB	1:C:230:VAL:HG13	2.02	0.41
1:B:138:VAL:O	1:B:138:VAL:CG1	2.68	0.41
1:A:138:VAL:O	1:A:138:VAL:CG1	2.68	0.41
1:C:48:ARG:NH1	1:C:94:PRO:HD3	2.36	0.41
1:E:48:ARG:NH1	1:E:94:PRO:HD3	2.36	0.41
1:E:142:ILE:CD1	1:E:188:VAL:HG22	2.51	0.41
1:E:232:VAL:CG1	1:E:234:GLN:HG2	2.50	0.41
1:C:232:VAL:CG1	1:C:234:GLN:HG2	2.50	0.41
1:E:243:LYS:O	1:E:243:LYS:HG2	2.21	0.40
1:B:38:MET:HE2	1:B:230:VAL:HB	2.03	0.40
1:B:92:GLY:C	1:B:94:PRO:HD3	2.46	0.40
1:C:107:TYR:CG	1:C:132:LEU:CD1	3.04	0.40
1:D:220:ILE:HB	1:D:230:VAL:HG13	2.02	0.40
1:D:251:TYR:O	1:D:252:ALA:HB2	2.22	0.40
1:D:268:GLU:HA	1:D:273:VAL:HG13	2.03	0.40
1:A:107:TYR:CD1	1:A:132:LEU:HD11	2.56	0.40
1:A:142:ILE:CD1	1:A:188:VAL:HG22	2.51	0.40
1:B:48:ARG:NH1	1:B:94:PRO:HD3	2.36	0.40
1:C:75:VAL:N	1:C:76:PRO:CD	2.84	0.40
1:D:102:LEU:HA	1:D:103:PRO:HD3	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/281 (87%)	231 (95%)	13 (5%)	0	100	100
1	B	244/281 (87%)	231 (95%)	13 (5%)	0	100	100
1	C	244/281 (87%)	232 (95%)	12 (5%)	0	100	100
1	D	244/281 (87%)	232 (95%)	12 (5%)	0	100	100
1	E	244/281 (87%)	231 (95%)	13 (5%)	0	100	100
All	All	1220/1405 (87%)	1157 (95%)	63 (5%)	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	177/202 (88%)	169 (96%)	8 (4%)	24	58
1	B	177/202 (88%)	170 (96%)	7 (4%)	28	63
1	C	177/202 (88%)	169 (96%)	8 (4%)	24	58
1	D	177/202 (88%)	170 (96%)	7 (4%)	28	63
1	E	177/202 (88%)	170 (96%)	7 (4%)	28	63
All	All	885/1010 (88%)	848 (96%)	37 (4%)	26	61

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	112	THR
1	A	188	VAL
1	A	244	THR
1	A	257	GLU
1	A	260	ARG
1	A	264	GLN
1	A	273	VAL
1	B	112	THR
1	B	188	VAL

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Mol	Chain	Res	Type
1	B	244	THR
1	B	257	GLU
1	B	260	ARG
1	B	264	GLN
1	B	273	VAL
1	C	40	THR
1	C	112	THR
1	C	188	VAL
1	C	244	THR
1	C	257	GLU
1	C	260	ARG
1	C	264	GLN
1	C	273	VAL
1	D	112	THR
1	D	188	VAL
1	D	244	THR
1	D	257	GLU
1	D	260	ARG
1	D	264	GLN
1	D	273	VAL
1	E	112	THR
1	E	188	VAL
1	E	244	THR
1	E	257	GLU
1	E	260	ARG
1	E	264	GLN
1	E	273	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	229	GLN
1	A	264	GLN
1	A	279	HIS
1	B	128	HIS
1	B	229	GLN
1	B	264	GLN
1	B	279	HIS
1	C	128	HIS
1	C	229	GLN
1	C	264	GLN

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Mol	Chain	Res	Type
1	C	279	HIS
1	D	128	HIS
1	D	229	GLN
1	D	264	GLN
1	D	279	HIS
1	E	128	HIS
1	E	229	GLN
1	E	264	GLN
1	E	279	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å ²)	Q<0.9
1	A	248/281 (88%)	0.22	13 (5%)	33	25	13, 30, 77, 113	0
1	B	248/281 (88%)	0.65	22 (8%)	15	11	15, 48, 92, 130	0
1	C	248/281 (88%)	0.58	25 (10%)	12	9	13, 44, 91, 134	0
1	D	248/281 (88%)	0.36	18 (7%)	21	15	14, 30, 77, 121	0
1	E	248/281 (88%)	0.64	22 (8%)	15	11	16, 43, 94, 138	0
All	All	1240/1405 (88%)	0.49	100 (8%)	18	13	13, 37, 89, 138	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	LYS	4.7
1	E	175	GLY	4.7
1	D	260	ARG	4.6
1	D	267	GLN	4.6
1	A	175	GLY	4.4
1	B	247	PHE	4.4
1	D	264	GLN	4.3
1	C	244	THR	4.3
1	E	244	THR	4.3
1	B	175	GLY	4.2
1	A	34	HIS	4.1
1	D	179	GLU	4.1
1	C	279	HIS	4.0
1	C	175	GLY	4.0
1	E	247	PHE	3.9
1	D	176	ASP	3.8
1	D	242	ALA	3.8
1	D	208	GLN	3.8
1	B	279	HIS	3.8
1	C	160	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	264	GLN	3.6
1	C	277	ASP	3.5
1	D	175	GLY	3.4
1	B	276	ALA	3.3
1	C	260	ARG	3.3
1	E	19	THR	3.2
1	A	278	GLU	3.2
1	B	244	THR	3.1
1	C	204	GLU	3.1
1	B	160	PRO	3.1
1	E	245	ALA	3.1
1	D	259	ARG	3.0
1	E	204	GLU	3.0
1	A	244	THR	3.0
1	C	274	PHE	3.0
1	B	260	ARG	3.0
1	C	278	GLU	3.0
1	E	278	GLU	3.0
1	E	241	GLY	2.9
1	B	259	ARG	2.9
1	B	240	SER	2.8
1	B	223	GLY	2.8
1	B	278	GLU	2.7
1	E	279	HIS	2.7
1	E	259	ARG	2.7
1	B	269	VAL	2.7
1	B	19	THR	2.7
1	E	243	LYS	2.6
1	C	250	ARG	2.6
1	E	212	LYS	2.6
1	C	211	GLY	2.6
1	E	242	ALA	2.6
1	A	245	ALA	2.5
1	D	246	ARG	2.5
1	C	208	GLN	2.5
1	D	243	LYS	2.5
1	D	241	GLY	2.5
1	A	259	ARG	2.4
1	C	246	ARG	2.4
1	C	247	PHE	2.4
1	A	242	ALA	2.4
1	C	262	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	233	TRP	2.3
1	D	244	THR	2.3
1	C	20	LYS	2.3
1	B	138	VAL	2.3
1	A	247	PHE	2.3
1	B	190	GLU	2.3
1	C	159	THR	2.3
1	D	159	THR	2.3
1	B	246	ARG	2.3
1	C	137	ARG	2.3
1	C	276	ALA	2.2
1	A	246	ARG	2.2
1	E	137	ARG	2.2
1	B	159	THR	2.2
1	D	204	GLU	2.2
1	D	276	ALA	2.2
1	B	34	HIS	2.2
1	E	34	HIS	2.2
1	B	204	GLU	2.2
1	B	224	PRO	2.2
1	A	243	LYS	2.2
1	C	215	ILE	2.1
1	D	214	THR	2.1
1	E	208	GLN	2.1
1	C	271	GLY	2.1
1	C	205	LEU	2.1
1	B	137	ARG	2.1
1	B	221	GLY	2.1
1	E	250	ARG	2.1
1	E	260	ARG	2.1
1	E	276	ALA	2.1
1	A	159	THR	2.1
1	E	182	ILE	2.1
1	E	201	VAL	2.0
1	A	73	THR	2.0
1	A	241	GLY	2.0
1	E	271	GLY	2.0
1	C	245	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	902	1/1	0.66	0.19	55,55,55,55	0
2	MG	C	903	1/1	0.78	0.21	52,52,52,52	0
2	MG	D	904	1/1	0.84	0.13	49,49,49,49	0
2	MG	A	901	1/1	0.89	0.12	48,48,48,48	0
2	MG	E	905	1/1	0.90	0.14	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.