



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:07 PM UTC

PDB ID : 3GAA / pdb_00003gaa
Title : The crystal structure of the protein with unknown function from *Thermoplasma acidophilum*
Authors : Zhang, R.; Borovilos, M.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-02-16
Resolution : 2.70 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

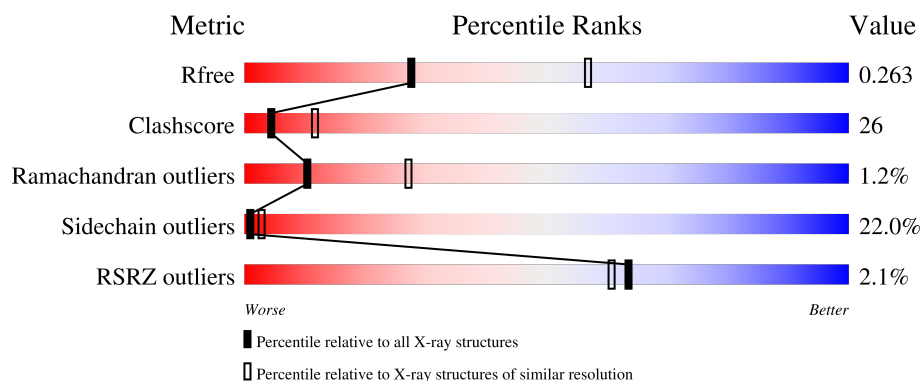
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	252	2% 54% 31% 11% • •
1	B	252	% 56% 27% 11% • •
1	C	252	% 52% 31% 11% • •
1	D	252	3% 53% 33% 10% •
1	E	252	3% 56% 27% 10% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9299 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 uncharacterized protein Ta1441.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1856	1183	310	352	11			
1	B	242	Total	C	N	O	S	0	0	0
			1848	1178	309	351	10			
1	C	243	Total	C	N	O	S	0	0	0
			1856	1183	310	352	11			
1	D	242	Total	C	N	O	S	0	0	0
			1848	1177	309	351	11			
1	E	243	Total	C	N	O	S	0	0	0
			1856	1183	310	352	11			

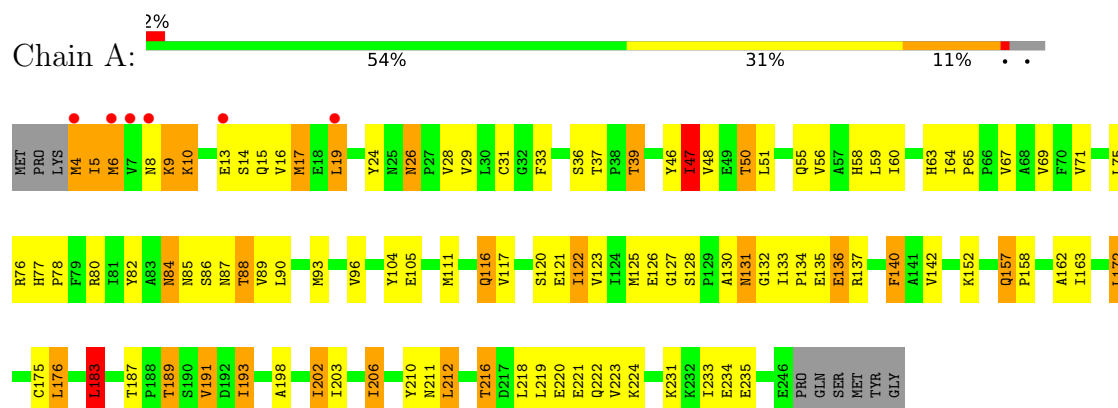
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	10	Total	O	0	0
			10	10		
2	C	6	Total	O	0	0
			6	6		
2	D	6	Total	O	0	0
			6	6		
2	E	3	Total	O	0	0
			3	3		

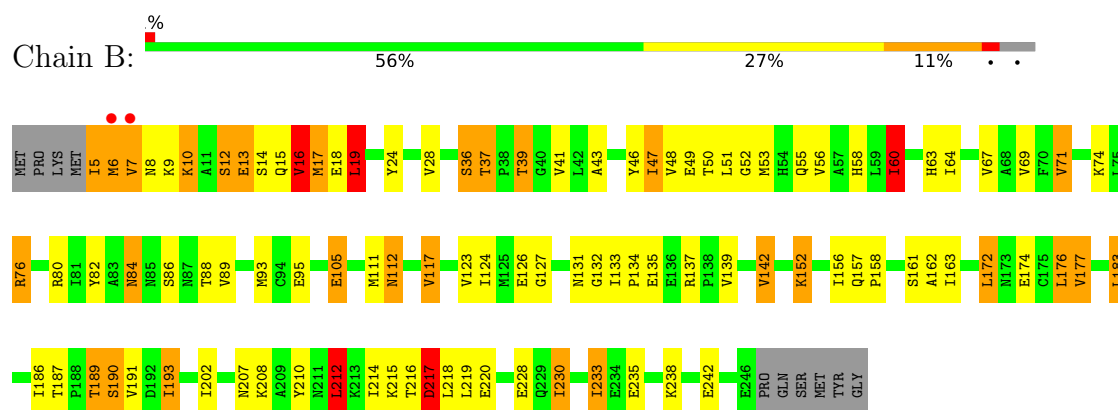
3 Residue-property plots

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.

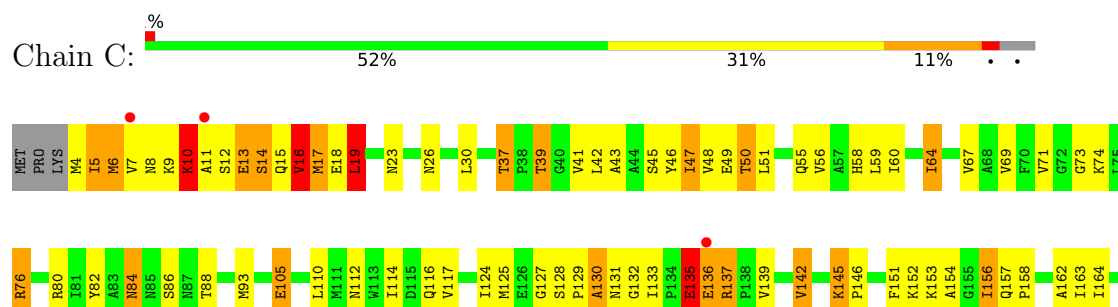
• Molecule 1: uncharacterized protein Ta1441



• Molecule 1: uncharacterized protein Ta1441

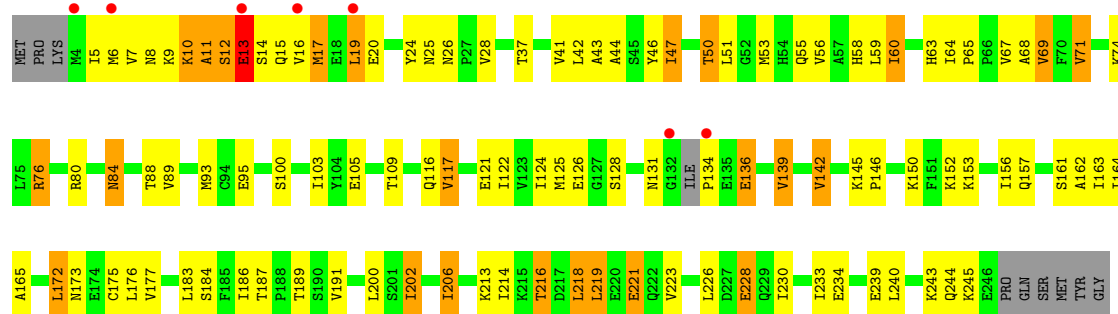


• Molecule 1: uncharacterized protein Ta1441

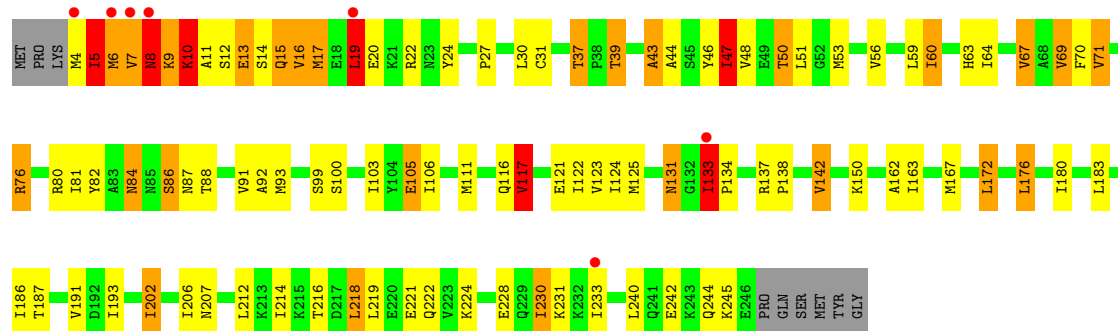




• Molecule 1: uncharacterized protein Ta1441



• Molecule 1: uncharacterized protein Ta1441



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.32Å 184.32Å 260.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.02 – 2.70 101.02 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (101.02-2.70) 99.7 (101.02-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.196 , 0.256 0.206 , 0.263	Depositor DCC
R_{free} test set	2363 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9299	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 4.97% 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	1.36	7/1888 (0.4%)	1.33	14/2558 (0.5%)
1	B	1.36	7/1880 (0.4%)	1.28	11/2548 (0.4%)
1	C	1.28	6/1888 (0.3%)	1.29	8/2558 (0.3%)
1	D	1.24	4/1879 (0.2%)	1.26	13/2543 (0.5%)
1	E	1.21	3/1888 (0.2%)	1.21	6/2558 (0.2%)
All	All	1.29	27/9423 (0.3%)	1.27	52/12765 (0.4%)

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	B	0	1
1	C	0	1
All	All	0	2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	16	VAL	CA-CB	8.57	1.65	1.54
1	B	16	VAL	CA-CB	8.51	1.63	1.54
1	C	193	ILE	CA-CB	6.77	1.63	1.53
1	A	47	ILE	CA-CB	6.43	1.62	1.54
1	E	5	ILE	N-CA	6.09	1.53	1.46
1	C	39	THR	CA-CB	5.98	1.62	1.53
1	B	193	ILE	CA-C	5.97	1.57	1.52
1	C	16	VAL	CA-CB	5.90	1.63	1.54
1	E	7	VAL	CA-CB	-5.80	1.46	1.54
1	B	142	VAL	CA-CB	5.75	1.61	1.54
1	C	6	MET	CB-CG	5.67	1.69	1.52
1	C	5	ILE	CA-CB	5.62	1.59	1.53
1	D	234	GLU	CG-CD	5.59	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	LEU	CA-C	-5.59	1.45	1.52
1	D	234	GLU	CB-CG	5.47	1.68	1.52
1	A	216	THR	N-CA	5.34	1.53	1.46
1	D	13	GLU	CG-CD	5.29	1.65	1.52
1	A	122	ILE	C-O	-5.29	1.18	1.24
1	E	47	ILE	CA-CB	5.27	1.61	1.54
1	B	60	ILE	CG1-CD1	5.23	1.72	1.51
1	B	112	ASN	CB-CG	-5.16	1.39	1.52
1	C	135	GLU	N-CA	5.15	1.52	1.46
1	B	191	VAL	CA-CB	5.10	1.60	1.54
1	B	216	THR	CA-C	5.09	1.59	1.52
1	A	140	PHE	CA-C	-5.07	1.46	1.52
1	A	206	ILE	CA-CB	-5.04	1.48	1.54
1	A	234	GLU	CG-CD	5.03	1.64	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	N-CA-C	-10.88	96.18	110.43
1	C	212	LEU	N-CA-C	-9.63	97.06	110.35
1	B	215	LYS	N-CA-C	9.24	121.12	111.14
1	D	16	VAL	N-CA-C	-8.15	102.30	110.62
1	B	212	LEU	N-CA-C	-7.89	99.47	110.35
1	D	136	GLU	N-CA-C	-7.72	98.03	109.15
1	E	8	ASN	N-CA-C	7.60	121.62	109.24
1	E	212	LEU	N-CA-C	-6.71	101.87	110.19
1	C	8	ASN	N-CA-C	6.63	119.14	107.61
1	B	193	ILE	N-CA-CB	-6.59	107.28	111.83
1	D	20	GLU	N-CA-C	6.55	119.24	111.71
1	A	234	GLU	N-CA-C	-6.47	103.34	111.11
1	D	65	PRO	CA-C-N	6.37	127.81	119.84
1	D	65	PRO	C-N-CA	6.37	127.81	119.84
1	B	16	VAL	N-CA-CB	6.24	117.44	110.51
1	B	19	LEU	N-CA-C	-6.20	103.01	111.56
1	E	133	ILE	CA-C-N	-6.18	113.59	119.90
1	E	133	ILE	C-N-CA	-6.18	113.59	119.90
1	A	128	SER	CA-C-N	-6.16	113.34	119.99
1	A	128	SER	C-N-CA	-6.16	113.34	119.99
1	B	233	ILE	N-CA-C	6.14	116.30	110.53
1	D	109	THR	N-CA-C	-6.04	104.61	111.14
1	A	126	GLU	N-CA-C	5.99	118.17	109.07
1	B	217	ASP	N-CA-C	-5.89	102.33	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-C-N	-5.70	115.39	123.03
1	A	212	LEU	C-N-CA	-5.70	115.39	123.03
1	B	64	ILE	N-CA-C	-5.67	101.36	108.05
1	A	26	ASN	N-CA-C	5.63	122.25	109.81
1	A	96	VAL	CA-C-N	-5.56	114.25	120.14
1	A	96	VAL	C-N-CA	-5.56	114.25	120.14
1	D	176	LEU	N-CA-C	-5.49	105.20	111.07
1	C	19	LEU	N-CA-C	-5.43	102.29	110.06
1	A	48	VAL	CB-CA-C	-5.36	105.02	111.88
1	D	175	CYS	N-CA-C	5.33	117.09	111.28
1	C	136	GLU	N-CA-C	-5.31	99.48	110.80
1	C	5	ILE	N-CA-C	5.31	114.43	106.42
1	D	12	SER	N-CA-C	-5.28	106.78	114.12
1	C	137	ARG	N-CA-C	-5.24	98.23	109.81
1	B	177	VAL	N-CA-C	5.23	115.96	110.62
1	D	68	ALA	CA-C-N	-5.23	115.44	122.91
1	D	68	ALA	C-N-CA	-5.23	115.44	122.91
1	D	128	SER	CA-C-N	-5.22	114.33	119.92
1	D	128	SER	C-N-CA	-5.22	114.33	119.92
1	E	19	LEU	N-CA-C	-5.22	104.18	110.44
1	E	43	ALA	N-CA-C	-5.21	105.49	111.07
1	A	216	THR	N-CA-C	5.18	121.60	113.72
1	A	235	GLU	N-CA-C	5.16	116.98	111.36
1	C	64	ILE	N-CA-C	-5.16	103.89	108.95
1	B	212	LEU	CA-C-N	-5.03	115.03	123.04
1	B	212	LEU	C-N-CA	-5.03	115.03	123.04
1	C	217	ASP	N-CA-C	-5.02	101.52	109.96
1	A	104	TYR	N-CA-C	5.01	117.13	111.11

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	7	VAL	Peptide
1	C	135	GLU	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	1856	0	1903	112	1
1	B	1848	0	1894	90	2
1	C	1856	0	1903	114	3
1	D	1848	0	1892	99	1
1	E	1856	0	1903	119	2
2	A	10	0	0	2	0
2	B	10	0	0	2	0
2	C	6	0	0	2	0
2	D	6	0	0	0	0
2	E	3	0	0	0	0
All	All	9299	0	9495	497	5

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 26.

All (497) 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:A:125:MET:HE3	1:A:206:ILE:CD1	1.66	1.24
1:D:125:MET:HE2	1:D:206:ILE:CD1	1.68	1.22
1:A:10:LYS:HB3	1:A:10:LYS:HZ3	1.02	1.17
1:C:6:MET:HE1	1:C:16:VAL:HG13	1.23	1.15
1:D:10:LYS:NZ	1:D:10:LYS:HB3	1.60	1.14
1:C:125:MET:HE2	1:C:206:ILE:CD1	1.76	1.14
1:C:177:VAL:HG11	1:D:60:ILE:HD11	1.16	1.11
1:D:47:ILE:HD12	1:D:47:ILE:C	1.76	1.11
1:B:177:VAL:HG11	1:C:60:ILE:HD11	1.17	1.10
1:D:10:LYS:HB3	1:D:10:LYS:HZ3	0.98	1.10
1:C:46:TYR:O	1:C:50:THR:HG23	1.54	1.07
1:E:125:MET:HE2	1:E:206:ILE:CD1	1.84	1.07
1:D:125:MET:HE2	1:D:206:ILE:HD13	1.29	1.07
1:E:15:GLN:HE21	1:E:15:GLN:C	1.61	1.07
1:B:132:GLY:HA3	2:B:261:HOH:O	1.54	1.05
1:C:125:MET:HE2	1:C:206:ILE:HD13	1.36	1.05
1:A:80:ARG:HH12	1:A:93:MET:HE3	1.18	1.03
1:C:6:MET:HE1	1:C:16:VAL:CG1	1.90	1.02
1:A:10:LYS:HB3	1:A:10:LYS:NZ	1.65	1.01
1:A:125:MET:HE3	1:A:206:ILE:HD11	1.01	0.98
1:A:131:ASN:N	1:A:131:ASN:HD22	1.52	0.98
1:E:125:MET:CE	1:E:206:ILE:HD13	1.95	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:VAL:CG1	1:C:60:ILE:HD11	1.93	0.96
1:D:177:VAL:HG21	1:E:60:ILE:HD11	1.48	0.96
1:B:207:ASN:OD1	1:B:214:ILE:HD12	1.65	0.95
1:D:47:ILE:HD12	1:D:47:ILE:O	1.65	0.94
1:C:133:ILE:HG21	1:C:137:ARG:NH1	1.83	0.94
1:C:177:VAL:HG11	1:D:60:ILE:CD1	1.98	0.93
1:A:10:LYS:HZ3	1:A:10:LYS:CB	1.81	0.93
1:C:135:GLU:C	1:C:137:ARG:H	1.75	0.93
1:B:10:LYS:O	1:B:13:GLU:CD	2.11	0.92
1:A:125:MET:CE	1:A:206:ILE:HD11	1.96	0.92
1:D:125:MET:CE	1:D:206:ILE:HD13	1.99	0.92
1:A:162:ALA:HB1	1:B:233:ILE:HG12	1.49	0.92
1:A:125:MET:CE	1:A:206:ILE:CD1	2.48	0.91
1:E:125:MET:CE	1:E:206:ILE:CD1	2.48	0.91
1:A:137:ARG:HB3	2:A:261:HOH:O	1.69	0.91
1:C:177:VAL:CG1	1:D:60:ILE:HD11	2.01	0.91
1:A:39:THR:CG2	1:A:189:THR:HG21	2.01	0.90
1:B:177:VAL:HG11	1:C:60:ILE:CD1	2.02	0.90
1:C:125:MET:HE2	1:C:206:ILE:HD11	1.51	0.89
1:E:8:ASN:N	1:E:8:ASN:HD22	1.64	0.89
1:D:71:VAL:HB	1:D:233:ILE:HD11	1.54	0.89
1:A:10:LYS:NZ	1:A:10:LYS:CB	2.30	0.89
1:C:59:LEU:CD2	1:C:64:ILE:HD11	2.02	0.88
1:B:163:ILE:CG2	1:C:233:ILE:HG23	2.04	0.88
1:D:10:LYS:NZ	1:D:10:LYS:CB	2.30	0.88
1:A:39:THR:HG21	1:A:189:THR:HG21	1.57	0.87
1:B:53:MET:HE1	1:B:89:VAL:HG12	1.57	0.86
1:D:125:MET:HE2	1:D:206:ILE:HD11	1.55	0.86
1:D:163:ILE:CG2	1:E:233:ILE:HG23	2.07	0.85
1:E:125:MET:HE2	1:E:206:ILE:HD13	1.54	0.85
1:C:47:ILE:HD12	1:C:47:ILE:O	1.77	0.84
1:C:82:TYR:CE2	1:C:93:MET:HE3	2.12	0.84
1:D:125:MET:CE	1:D:206:ILE:CD1	2.53	0.84
1:E:84:ASN:C	1:E:84:ASN:HD22	1.85	0.84
1:A:162:ALA:HB1	1:B:233:ILE:CG1	2.08	0.83
1:C:152:LYS:NZ	1:C:157:GLN:HE21	1.75	0.83
1:A:233:ILE:HG12	1:E:162:ALA:HB1	1.58	0.83
1:C:59:LEU:HD23	1:C:64:ILE:HD11	1.58	0.83
1:E:47:ILE:CD1	1:E:51:LEU:HD12	2.09	0.83
1:D:84:ASN:HD21	1:D:88:THR:H	1.27	0.83
1:E:19:LEU:O	1:E:19:LEU:HD23	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:LYS:NZ	1:C:157:GLN:NE2	2.28	0.82
1:C:152:LYS:HZ1	1:C:157:GLN:NE2	1.77	0.82
1:D:136:GLU:HG3	1:D:136:GLU:O	1.78	0.82
1:E:125:MET:HE2	1:E:206:ILE:HD11	1.61	0.82
1:A:8:ASN:ND2	1:A:16:VAL:HG21	1.99	0.78
1:D:10:LYS:O	1:D:11:ALA:CB	2.32	0.78
1:E:7:VAL:C	1:E:8:ASN:HD22	1.91	0.78
1:B:71:VAL:HG12	1:B:76:ARG:HH12	1.48	0.77
1:B:39:THR:CG2	1:B:189:THR:HG21	2.14	0.77
1:B:71:VAL:HB	1:B:233:ILE:HD11	1.67	0.76
1:D:10:LYS:O	1:D:11:ALA:HB3	1.84	0.76
1:B:53:MET:CE	1:B:89:VAL:HG12	2.14	0.76
1:C:162:ALA:HB1	1:D:233:ILE:CG1	2.15	0.76
1:B:43:ALA:O	1:B:47:ILE:HG23	1.86	0.76
1:A:46:TYR:CE1	1:A:50:THR:HG21	2.22	0.75
1:C:162:ALA:HB1	1:D:233:ILE:HG12	1.69	0.75
1:E:46:TYR:O	1:E:50:THR:HG23	1.85	0.75
1:E:63:HIS:ND1	1:E:105:GLU:OE2	2.20	0.75
1:D:162:ALA:HB1	1:E:233:ILE:CG1	2.17	0.75
1:D:44:ALA:HB1	1:D:93:MET:HE2	1.68	0.74
1:C:214:ILE:O	1:C:216:THR:HG23	1.88	0.74
1:E:15:GLN:C	1:E:15:GLN:NE2	2.43	0.74
1:B:163:ILE:HG21	1:C:233:ILE:HG23	1.70	0.74
1:D:24:TYR:CD2	1:D:117:VAL:HG22	2.23	0.73
1:C:30:LEU:HD13	1:C:125:MET:HE1	1.71	0.73
1:D:136:GLU:O	1:D:136:GLU:CG	2.35	0.73
1:E:84:ASN:HD21	1:E:88:THR:H	1.36	0.73
1:A:80:ARG:NH1	1:A:93:MET:HE3	2.01	0.73
1:A:122:ILE:HD12	1:A:175:CYS:SG	2.28	0.73
1:B:10:LYS:O	1:B:13:GLU:OE2	2.06	0.73
1:A:233:ILE:CG1	1:E:162:ALA:HB1	2.17	0.73
1:C:6:MET:CE	1:C:16:VAL:HG13	2.13	0.73
1:C:55:GLN:HE22	1:C:58:HIS:CE1	2.06	0.72
1:B:55:GLN:HE22	1:B:58:HIS:CE1	2.05	0.72
1:A:55:GLN:HE22	1:A:58:HIS:CE1	2.07	0.71
1:E:63:HIS:CE1	1:E:105:GLU:OE2	2.43	0.71
1:E:133:ILE:HG23	1:E:134:PRO:HD2	1.73	0.71
1:B:84:ASN:C	1:B:84:ASN:HD22	1.98	0.71
1:A:46:TYR:CZ	1:A:50:THR:HG21	2.24	0.71
1:C:5:ILE:O	1:C:5:ILE:HG22	1.88	0.71
1:D:47:ILE:C	1:D:47:ILE:CD1	2.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:O	1:C:137:ARG:N	2.19	0.71
1:A:8:ASN:HD22	1:A:16:VAL:HG11	1.56	0.71
1:C:84:ASN:HD21	1:C:88:THR:H	1.37	0.71
1:E:10:LYS:C	1:E:12:SER:H	1.98	0.71
1:B:6:MET:HE1	1:B:16:VAL:CG1	2.21	0.71
1:A:84:ASN:HD21	1:A:88:THR:H	1.38	0.70
1:C:135:GLU:C	1:C:137:ARG:N	2.35	0.70
1:D:162:ALA:HB1	1:E:233:ILE:HG13	1.74	0.70
1:B:24:TYR:CD2	1:B:117:VAL:HG22	2.25	0.70
1:C:6:MET:CE	1:C:16:VAL:CG1	2.70	0.70
1:E:8:ASN:N	1:E:8:ASN:ND2	2.35	0.69
1:B:6:MET:HE1	1:B:16:VAL:HG11	1.74	0.69
1:A:6:MET:SD	1:A:16:VAL:HG13	2.33	0.68
1:C:10:LYS:O	1:C:13:GLU:OE1	2.11	0.68
1:B:46:TYR:CZ	1:B:50:THR:HG21	2.28	0.68
1:A:4:MET:CG	1:A:5:ILE:HD13	2.24	0.68
1:C:59:LEU:HD23	1:C:64:ILE:CD1	2.23	0.68
1:E:131:ASN:HD21	1:E:133:ILE:CD1	2.07	0.68
1:B:162:ALA:HB1	1:C:233:ILE:CG1	2.24	0.68
1:A:39:THR:HG23	1:A:189:THR:HG21	1.76	0.68
1:A:8:ASN:ND2	1:A:16:VAL:HG11	2.09	0.67
1:E:131:ASN:ND2	1:E:133:ILE:CD1	2.57	0.67
1:E:47:ILE:HD12	1:E:47:ILE:O	1.95	0.67
1:A:63:HIS:ND1	1:A:105:GLU:OE2	2.28	0.67
1:D:46:TYR:O	1:D:50:THR:HG23	1.94	0.67
1:D:47:ILE:HD13	1:D:51:LEU:HD12	1.77	0.67
1:D:163:ILE:HG21	1:E:233:ILE:HG23	1.76	0.67
1:B:80:ARG:NH2	1:B:95:GLU:OE1	2.28	0.67
1:D:46:TYR:CZ	1:D:50:THR:HG21	2.30	0.67
1:D:55:GLN:HE22	1:D:58:HIS:CE1	2.11	0.66
1:D:219:LEU:C	1:D:219:LEU:HD23	2.20	0.66
1:E:6:MET:SD	1:E:16:VAL:CG2	2.84	0.66
1:A:131:ASN:HD22	1:A:131:ASN:H	1.40	0.66
1:B:37:THR:HG21	1:B:127:GLY:C	2.20	0.66
1:D:10:LYS:CB	1:D:10:LYS:HZ2	2.09	0.66
1:E:125:MET:CE	1:E:206:ILE:HD11	2.21	0.66
1:C:133:ILE:HG21	1:C:137:ARG:HH12	1.60	0.65
1:D:71:VAL:HG12	1:D:76:ARG:HH12	1.61	0.65
1:C:47:ILE:HD12	1:C:47:ILE:C	2.21	0.65
1:D:218:LEU:HD13	1:D:218:LEU:N	2.11	0.65
1:C:19:LEU:O	1:C:19:LEU:HD23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:CD1	1:E:172:LEU:HD13	2.26	0.65
1:B:163:ILE:HG23	1:C:233:ILE:HG23	1.78	0.64
1:C:59:LEU:HD22	1:C:64:ILE:HD11	1.78	0.64
1:C:214:ILE:O	1:C:216:THR:CG2	2.45	0.64
1:E:10:LYS:O	1:E:12:SER:N	2.30	0.64
1:B:47:ILE:HD12	1:B:47:ILE:C	2.21	0.64
1:E:5:ILE:HG22	1:E:5:ILE:O	1.96	0.64
1:E:46:TYR:CZ	1:E:50:THR:HG21	2.33	0.64
1:E:53:MET:HE1	1:E:91:VAL:HG23	1.78	0.64
1:E:218:LEU:HG	1:E:221:GLU:HB2	1.78	0.64
1:C:125:MET:CE	1:C:206:ILE:HD13	2.23	0.64
1:E:71:VAL:HB	1:E:233:ILE:HD11	1.80	0.63
1:B:7:VAL:CG1	1:B:8:ASN:H	2.11	0.63
1:A:131:ASN:N	1:A:131:ASN:ND2	2.28	0.63
1:D:43:ALA:O	1:D:47:ILE:HG23	1.99	0.63
1:E:131:ASN:HD21	1:E:133:ILE:HD11	1.63	0.63
1:A:6:MET:SD	1:A:16:VAL:CG1	2.86	0.63
1:A:193:ILE:HD13	1:A:193:ILE:H	1.62	0.63
1:B:39:THR:HG21	1:B:189:THR:HG21	1.80	0.62
1:E:106:ILE:HB	1:E:167:MET:HE1	1.80	0.62
1:A:71:VAL:HB	1:A:233:ILE:HD11	1.82	0.62
1:C:47:ILE:CD1	1:C:51:LEU:HD12	2.30	0.62
1:B:133:ILE:HG23	1:B:134:PRO:HD2	1.82	0.62
1:B:162:ALA:HB1	1:C:233:ILE:HG12	1.80	0.62
1:E:131:ASN:ND2	1:E:133:ILE:HD13	2.14	0.61
1:B:157:GLN:HB2	1:B:158:PRO:CD	2.31	0.61
1:D:162:ALA:HB1	1:E:233:ILE:HG12	1.81	0.61
1:A:130:ALA:HB3	1:A:133:ILE:HD11	1.82	0.61
1:E:6:MET:SD	1:E:16:VAL:HG22	2.41	0.61
1:E:84:ASN:C	1:E:84:ASN:ND2	2.54	0.61
1:B:152:LYS:HZ1	1:B:158:PRO:HD3	1.65	0.60
1:C:127:GLY:HA3	1:C:189:THR:HG21	1.82	0.60
1:D:14:SER:HA	1:D:19:LEU:HD22	1.84	0.60
1:C:30:LEU:HB3	1:C:125:MET:HE3	1.82	0.60
1:E:59:LEU:CD2	1:E:64:ILE:HD11	2.32	0.60
1:A:39:THR:HG21	1:A:189:THR:CG2	2.30	0.60
1:E:14:SER:HA	1:E:19:LEU:HD22	1.84	0.60
1:E:6:MET:SD	1:E:16:VAL:HG21	2.42	0.60
1:D:84:ASN:HD21	1:D:88:THR:N	1.99	0.59
1:A:163:ILE:CG2	1:B:233:ILE:HG23	2.32	0.59
1:C:152:LYS:HZ3	1:C:157:GLN:HE21	1.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:ILE:HD12	1:E:47:ILE:C	2.28	0.59
1:A:111:MET:SD	1:A:122:ILE:HD13	2.43	0.59
1:B:7:VAL:CG1	1:B:8:ASN:N	2.66	0.59
1:E:59:LEU:HD22	1:E:64:ILE:HD11	1.83	0.59
1:B:10:LYS:O	1:B:13:GLU:OE1	2.20	0.58
1:C:14:SER:HA	1:C:19:LEU:HD22	1.84	0.58
1:E:15:GLN:NE2	1:E:15:GLN:O	2.33	0.58
1:A:46:TYR:O	1:A:50:THR:HG23	2.04	0.58
1:C:129:PRO:HB3	1:C:191:VAL:HG22	1.85	0.58
1:B:217:ASP:O	1:B:218:LEU:HB2	2.02	0.58
1:D:55:GLN:NE2	1:D:58:HIS:CE1	2.72	0.58
1:D:100:SER:HA	1:D:103:ILE:HD12	1.86	0.58
1:B:14:SER:OG	1:B:19:LEU:CD2	2.52	0.58
1:E:43:ALA:O	1:E:47:ILE:HG23	2.04	0.57
1:C:162:ALA:HB1	1:D:233:ILE:HG13	1.85	0.57
1:D:47:ILE:CD1	1:D:51:LEU:HD12	2.34	0.57
1:B:157:GLN:HB2	1:B:158:PRO:HD2	1.87	0.57
1:D:228:GLU:HA	1:D:228:GLU:OE1	2.05	0.57
1:E:15:GLN:HE21	1:E:15:GLN:CA	2.17	0.57
1:B:14:SER:OG	1:B:19:LEU:HD23	2.05	0.57
1:E:80:ARG:NH1	1:E:82:TYR:OH	2.37	0.57
1:A:46:TYR:O	1:A:50:THR:CG2	2.53	0.57
1:A:47:ILE:CD1	1:A:51:LEU:HD12	2.35	0.57
1:A:211:ASN:C	1:A:212:LEU:O	2.42	0.56
1:A:132:GLY:CA	1:A:133:ILE:HD12	2.35	0.56
1:C:124:ILE:CD1	1:C:172:LEU:HD13	2.35	0.56
1:D:139:VAL:CG1	1:D:156:ILE:HD13	2.36	0.56
1:C:246:GLU:HB3	2:C:258:HOH:O	2.06	0.56
1:E:125:MET:HE3	1:E:206:ILE:CD1	2.35	0.56
1:B:43:ALA:O	1:B:47:ILE:CG2	2.53	0.56
1:E:10:LYS:O	1:E:13:GLU:HG2	2.06	0.56
1:C:214:ILE:O	1:C:215:LYS:C	2.49	0.56
1:D:17:MET:HE3	1:D:17:MET:HA	1.88	0.55
1:B:47:ILE:HD12	1:B:47:ILE:O	2.05	0.55
1:C:30:LEU:HD13	1:C:125:MET:CE	2.34	0.55
1:C:84:ASN:C	1:C:84:ASN:HD22	2.15	0.55
1:D:125:MET:CE	1:D:206:ILE:HD11	2.26	0.55
1:D:139:VAL:HG12	1:D:156:ILE:HD13	1.89	0.55
1:E:142:VAL:CG1	1:E:186:ILE:HD11	2.37	0.55
1:A:4:MET:N	1:A:4:MET:HE2	2.21	0.55
1:C:55:GLN:NE2	1:C:58:HIS:CE1	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HH12	1:A:93:MET:CE	2.07	0.55
1:C:145:LYS:HB3	1:C:146:PRO:HD3	1.88	0.55
1:D:177:VAL:CG2	1:E:60:ILE:HD11	2.31	0.55
1:D:218:LEU:N	1:D:218:LEU:CD1	2.70	0.55
1:E:207:ASN:HD21	1:E:214:ILE:HB	1.72	0.55
1:D:142:VAL:HG13	1:D:184:SER:HB3	1.89	0.54
1:E:122:ILE:HD12	1:E:180:ILE:HG21	1.89	0.54
1:C:10:LYS:C	1:C:12:SER:H	2.16	0.54
1:E:17:MET:HB3	1:E:19:LEU:HB3	1.88	0.54
1:C:14:SER:N	1:C:19:LEU:HD22	2.23	0.54
1:E:221:GLU:OE2	1:E:221:GLU:HA	2.08	0.54
1:A:134:PRO:O	1:A:136:GLU:N	2.40	0.54
1:D:59:LEU:CD2	1:D:64:ILE:HD11	2.38	0.54
1:B:124:ILE:CD1	1:B:172:LEU:HD13	2.39	0.54
1:B:162:ALA:HB1	1:C:233:ILE:HG13	1.88	0.53
1:C:151:PHE:HA	1:C:154:ALA:HB3	1.89	0.53
1:D:134:PRO:HB2	1:D:136:GLU:O	2.08	0.53
1:B:84:ASN:C	1:B:84:ASN:ND2	2.65	0.53
1:A:116:GLN:HE21	1:A:116:GLN:CA	2.20	0.53
1:A:5:ILE:O	1:A:5:ILE:HG22	2.07	0.53
1:C:133:ILE:HD11	1:C:190:SER:OG	2.08	0.53
1:A:111:MET:HE1	1:A:122:ILE:HD11	1.91	0.53
1:E:4:MET:SD	1:E:5:ILE:HD13	2.49	0.53
1:A:14:SER:HA	1:A:19:LEU:HD22	1.90	0.53
1:A:4:MET:HG3	1:A:5:ILE:HD13	1.91	0.52
1:A:222:GLN:NE2	2:A:260:HOH:O	2.36	0.52
1:D:59:LEU:HD23	1:D:64:ILE:HD11	1.91	0.52
1:D:42:LEU:CD2	1:D:226:LEU:HB3	2.39	0.52
1:A:123:VAL:HG13	1:A:183:LEU:CD2	2.39	0.52
1:C:157:GLN:HB2	1:C:158:PRO:HD2	1.92	0.52
1:E:10:LYS:C	1:E:12:SER:N	2.59	0.52
1:D:14:SER:CA	1:D:19:LEU:HD22	2.39	0.52
1:A:163:ILE:HG23	1:B:233:ILE:HG23	1.92	0.52
1:A:133:ILE:O	1:A:134:PRO:C	2.51	0.52
1:B:16:VAL:HG12	1:B:17:MET:HE3	1.92	0.52
1:E:10:LYS:N	1:E:10:LYS:CD	2.70	0.52
1:A:140:PHE:HA	1:A:157:GLN:O	2.09	0.52
1:B:47:ILE:CD1	1:B:51:LEU:HD12	2.39	0.52
1:C:10:LYS:O	1:C:12:SER:N	2.42	0.51
1:C:137:ARG:HG2	1:C:188:PRO:HD2	1.92	0.51
1:E:46:TYR:CE1	1:E:219:LEU:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:VAL:HG12	1:D:76:ARG:NH1	2.25	0.51
1:D:202:ILE:HG23	1:D:206:ILE:HD12	1.91	0.51
1:A:125:MET:CE	1:A:206:ILE:HD12	2.35	0.51
1:B:139:VAL:O	1:B:156:ILE:HG23	2.10	0.51
1:C:6:MET:SD	1:C:16:VAL:CG2	2.98	0.51
1:E:59:LEU:C	1:E:59:LEU:HD23	2.36	0.51
1:D:163:ILE:O	1:D:164:ILE:HD13	2.11	0.51
1:B:12:SER:O	1:B:13:GLU:C	2.51	0.51
1:B:123:VAL:HG13	1:B:183:LEU:CD2	2.41	0.51
1:C:14:SER:CA	1:C:19:LEU:HD22	2.40	0.51
1:C:137:ARG:NH2	1:C:195:ASP:OD1	2.44	0.51
1:C:10:LYS:O	1:C:13:GLU:CD	2.54	0.51
1:D:69:VAL:HG22	1:D:76:ARG:CZ	2.41	0.51
1:E:122:ILE:CD1	1:E:180:ILE:HG21	2.41	0.51
1:C:152:LYS:O	1:C:153:LYS:C	2.54	0.51
1:E:10:LYS:O	1:E:13:GLU:OE1	2.29	0.51
1:E:124:ILE:HD11	1:E:172:LEU:HD13	1.93	0.50
1:E:187:THR:CG2	1:E:202:ILE:CD1	2.88	0.50
1:E:125:MET:HE3	1:E:206:ILE:HD13	1.87	0.50
1:B:7:VAL:HG13	1:B:8:ASN:H	1.75	0.50
1:A:183:LEU:HD11	1:A:210:TYR:OH	2.11	0.50
1:B:7:VAL:HG12	1:B:8:ASN:N	2.26	0.50
1:B:84:ASN:HD21	1:B:88:THR:H	1.58	0.50
1:E:43:ALA:O	1:E:47:ILE:CG2	2.60	0.50
1:A:64:ILE:O	1:A:65:PRO:C	2.53	0.50
1:C:5:ILE:O	1:C:5:ILE:CG2	2.57	0.50
1:D:163:ILE:HG23	1:E:233:ILE:HG23	1.91	0.50
1:D:200:LEU:HD13	1:D:219:LEU:HD13	1.93	0.50
1:A:84:ASN:HD21	1:A:88:THR:N	2.07	0.50
1:A:183:LEU:C	1:A:183:LEU:HD22	2.37	0.50
1:A:162:ALA:HB1	1:B:233:ILE:HG13	1.90	0.49
1:D:126:GLU:O	1:D:186:ILE:HA	2.12	0.49
1:D:100:SER:HA	1:D:103:ILE:CD1	2.42	0.49
1:E:30:LEU:HD23	1:E:123:VAL:HB	1.93	0.49
1:C:187:THR:CG2	1:C:202:ILE:CD1	2.91	0.49
1:B:212:LEU:N	1:B:212:LEU:HD23	2.27	0.49
1:E:19:LEU:HG	1:E:22:ARG:HD2	1.93	0.49
1:C:46:TYR:CZ	1:C:50:THR:HG21	2.48	0.49
1:D:47:ILE:HD13	1:D:51:LEU:CD1	2.41	0.49
1:C:82:TYR:HE2	1:C:93:MET:HE3	1.71	0.49
1:D:69:VAL:HG22	1:D:76:ARG:NE	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:NH1	1:A:82:TYR:OH	2.47	0.48
1:A:233:ILE:HG23	1:E:163:ILE:CG2	2.43	0.48
1:D:214:ILE:O	1:D:216:THR:HG23	2.14	0.48
1:C:48:VAL:HG21	1:C:93:MET:CE	2.43	0.48
1:C:133:ILE:N	1:C:133:ILE:HD12	2.29	0.48
1:A:8:ASN:ND2	1:A:16:VAL:CG2	2.74	0.48
1:B:132:GLY:CA	2:B:261:HOH:O	2.32	0.48
1:D:228:GLU:OE1	1:D:228:GLU:CA	2.61	0.48
1:C:154:ALA:HB1	1:C:208:LYS:CE	2.43	0.48
1:E:10:LYS:HD2	1:E:10:LYS:HA	1.32	0.48
1:A:82:TYR:CE2	1:A:93:MET:HE2	2.48	0.48
1:E:84:ASN:ND2	1:E:87:ASN:N	2.61	0.48
1:D:28:VAL:HG12	1:D:89:VAL:HG22	1.96	0.47
1:C:6:MET:CE	1:C:16:VAL:HG11	2.45	0.47
1:D:122:ILE:HD12	1:D:122:ILE:N	2.30	0.47
1:A:84:ASN:ND2	1:A:89:VAL:H	2.12	0.47
1:A:116:GLN:HE21	1:A:116:GLN:HA	1.80	0.47
1:A:221:GLU:OE1	1:A:224:LYS:NZ	2.43	0.47
1:E:84:ASN:HD21	1:E:87:ASN:N	2.13	0.47
1:C:10:LYS:HZ3	1:C:10:LYS:HG3	1.43	0.47
1:C:14:SER:HA	1:C:19:LEU:CD2	2.44	0.47
1:D:146:PRO:C	1:D:150:LYS:HZ2	2.23	0.47
1:B:152:LYS:NZ	1:B:158:PRO:HD3	2.30	0.47
1:B:172:LEU:O	1:B:176:LEU:HD22	2.15	0.47
1:C:6:MET:SD	1:C:16:VAL:HG21	2.53	0.47
1:C:129:PRO:CB	1:C:191:VAL:HG22	2.45	0.47
1:D:124:ILE:HD11	1:D:172:LEU:HD13	1.97	0.47
1:E:84:ASN:HD21	1:E:88:THR:N	2.08	0.47
1:E:133:ILE:CG2	1:E:134:PRO:HD2	2.43	0.47
1:A:130:ALA:O	1:A:191:VAL:HG22	2.14	0.47
1:A:183:LEU:CD2	1:A:183:LEU:C	2.88	0.47
1:B:230:ILE:N	1:B:230:ILE:CD1	2.78	0.47
1:C:221:GLU:N	1:C:221:GLU:OE1	2.47	0.47
1:A:132:GLY:N	1:A:133:ILE:HD12	2.29	0.47
1:D:219:LEU:CD2	1:D:223:VAL:HG21	2.45	0.47
1:A:8:ASN:HD21	1:A:16:VAL:CB	2.27	0.46
1:A:9:LYS:HB3	1:A:9:LYS:HE2	1.28	0.46
1:A:212:LEU:N	1:A:212:LEU:HD23	2.30	0.46
1:B:37:THR:OG1	1:B:39:THR:HG23	2.15	0.46
1:C:190:SER:O	1:C:192:ASP:N	2.48	0.46
1:E:10:LYS:HA	1:E:13:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:SD	1:A:122:ILE:CD1	3.03	0.46
1:B:163:ILE:CG2	1:C:233:ILE:CG2	2.87	0.46
1:E:84:ASN:ND2	1:E:88:THR:H	2.10	0.46
1:A:63:HIS:CE1	1:A:105:GLU:OE2	2.68	0.46
1:B:39:THR:HG21	1:B:189:THR:CG2	2.44	0.46
1:B:55:GLN:NE2	1:B:58:HIS:CE1	2.79	0.46
1:A:233:ILE:HG13	1:E:162:ALA:HB1	1.98	0.46
1:E:19:LEU:O	1:E:19:LEU:CD2	2.59	0.46
1:E:47:ILE:HD13	1:E:51:LEU:HD12	1.91	0.46
1:D:10:LYS:H	1:D:10:LYS:HG2	1.15	0.46
1:E:230:ILE:CD1	1:E:230:ILE:N	2.78	0.46
1:D:63:HIS:ND1	1:D:105:GLU:OE2	2.49	0.46
1:A:4:MET:HG2	1:A:5:ILE:N	2.31	0.45
1:A:77:HIS:CG	1:A:78:PRO:HD2	2.51	0.45
1:A:172:LEU:HD12	1:A:172:LEU:HA	1.76	0.45
1:B:124:ILE:HD12	1:B:172:LEU:HD13	1.98	0.45
1:B:71:VAL:HG12	1:B:76:ARG:NH1	2.24	0.45
1:D:28:VAL:HG23	1:D:121:GLU:HB2	1.98	0.45
1:D:84:ASN:C	1:D:84:ASN:HD22	2.24	0.45
1:C:128:SER:O	1:C:188:PRO:HA	2.16	0.45
1:B:51:LEU:O	1:B:52:GLY:C	2.58	0.45
1:D:161:SER:O	1:E:70:PHE:HB3	2.16	0.45
1:C:154:ALA:HB1	1:C:208:LYS:HE3	1.97	0.45
1:C:190:SER:OG	1:C:193:ILE:HD13	2.16	0.45
1:E:133:ILE:O	1:E:134:PRO:C	2.60	0.45
1:A:187:THR:HB	1:A:202:ILE:CD1	2.46	0.45
1:B:82:TYR:CE2	1:B:93:MET:HE3	2.52	0.45
1:A:75:LEU:HG	1:E:176:LEU:HD21	1.98	0.45
1:A:172:LEU:O	1:A:176:LEU:HD22	2.17	0.45
1:B:39:THR:HG23	1:B:189:THR:HG21	1.95	0.45
1:C:71:VAL:HG12	1:C:76:ARG:NH1	2.32	0.45
1:E:111:MET:HE1	1:E:180:ILE:HD12	1.99	0.45
1:A:189:THR:HB	1:A:198:ALA:HB2	1.99	0.45
1:B:127:GLY:HA3	1:B:189:THR:CG2	2.47	0.45
1:C:16:VAL:HG12	1:C:17:MET:SD	2.56	0.45
1:C:139:VAL:O	1:C:156:ILE:HG23	2.16	0.45
1:E:69:VAL:HG23	1:E:233:ILE:HD11	1.97	0.45
1:C:30:LEU:HD22	1:C:125:MET:HE3	1.99	0.45
1:C:142:VAL:CG1	1:C:186:ILE:HD11	2.47	0.45
1:E:137:ARG:HA	1:E:138:PRO:HD3	1.90	0.45
1:A:46:TYR:OH	1:A:216:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:HIS:ND1	1:B:105:GLU:OE2	2.48	0.45
1:A:47:ILE:HG22	1:A:203:ILE:HD11	1.98	0.44
1:E:44:ALA:O	1:E:48:VAL:HG23	2.17	0.44
1:D:14:SER:CB	1:D:19:LEU:HD22	2.46	0.44
1:B:6:MET:HE1	1:B:16:VAL:HG13	1.96	0.44
1:D:37:THR:HG21	1:D:189:THR:CG2	2.47	0.44
1:D:80:ARG:HH22	1:D:95:GLU:CD	2.26	0.44
1:E:9:LYS:HE3	1:E:9:LYS:HB2	1.43	0.44
1:A:189:THR:HB	1:A:198:ALA:CB	2.48	0.44
1:B:60:ILE:HD13	1:B:60:ILE:HA	1.84	0.44
1:C:129:PRO:O	1:C:130:ALA:HB2	2.17	0.44
1:B:19:LEU:HD23	1:B:19:LEU:O	2.18	0.44
1:D:243:LYS:C	1:D:245:LYS:H	2.25	0.44
1:E:48:VAL:HG21	1:E:93:MET:CE	2.48	0.44
1:E:124:ILE:CD1	1:E:172:LEU:CD1	2.94	0.44
1:A:37:THR:HG21	1:A:127:GLY:C	2.43	0.44
1:A:60:ILE:HD13	1:A:60:ILE:HG21	1.58	0.44
1:E:86:SER:HB2	1:E:88:THR:OG1	2.17	0.44
1:C:43:ALA:O	1:C:47:ILE:HG23	2.17	0.44
1:A:152:LYS:HE2	1:A:158:PRO:HD3	1.99	0.43
1:A:183:LEU:HD13	1:A:183:LEU:N	2.33	0.43
1:C:80:ARG:NH1	1:C:82:TYR:OH	2.51	0.43
1:C:130:ALA:O	1:C:190:SER:HA	2.18	0.43
1:E:106:ILE:N	1:E:106:ILE:HD13	2.32	0.43
1:E:214:ILE:O	1:E:216:THR:HG23	2.18	0.43
1:C:125:MET:CE	1:C:206:ILE:HD11	2.37	0.43
1:C:163:ILE:O	1:C:164:ILE:HD13	2.18	0.43
1:C:210:TYR:O	1:C:211:ASN:C	2.61	0.43
1:E:133:ILE:HG13	1:E:134:PRO:CD	2.48	0.43
1:A:17:MET:HE3	1:A:17:MET:HA	1.99	0.43
1:B:127:GLY:HA3	1:B:189:THR:HG21	1.99	0.43
1:C:43:ALA:O	1:C:47:ILE:CG2	2.66	0.43
1:D:173:ASN:HD21	1:E:67:VAL:C	2.25	0.43
1:B:230:ILE:N	1:B:230:ILE:HD13	2.34	0.43
1:C:86:SER:O	1:C:88:THR:HG23	2.19	0.43
1:E:46:TYR:CE1	1:E:50:THR:HG21	2.54	0.43
1:A:127:GLY:HA3	1:A:189:THR:CG2	2.48	0.43
1:D:239:GLU:O	1:D:240:LEU:C	2.61	0.43
1:A:59:LEU:HD22	1:A:64:ILE:HD11	2.01	0.43
1:C:130:ALA:HB1	2:C:254:HOH:O	2.18	0.43
1:C:163:ILE:C	1:C:164:ILE:HD13	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:GLU:HG2	1:E:13:GLU:H	1.42	0.43
1:E:31:CYS:HA	1:E:92:ALA:O	2.19	0.43
1:C:152:LYS:HA	1:C:156:ILE:O	2.18	0.43
1:E:70:PHE:O	1:E:70:PHE:CG	2.72	0.43
1:A:37:THR:HG21	1:A:189:THR:HG23	2.01	0.43
1:A:46:TYR:CZ	1:A:219:LEU:HD12	2.54	0.43
1:C:37:THR:HG21	1:C:127:GLY:O	2.19	0.43
1:C:110:LEU:HG	1:C:114:ILE:HD12	2.00	0.43
1:E:69:VAL:HG13	1:E:76:ARG:HD2	2.00	0.43
1:D:69:VAL:CG2	1:D:76:ARG:CZ	2.97	0.42
1:E:10:LYS:HZ3	1:E:10:LYS:HG3	1.37	0.42
1:A:6:MET:SD	1:A:16:VAL:HG11	2.58	0.42
1:A:8:ASN:HD21	1:A:16:VAL:HB	1.84	0.42
1:B:133:ILE:HG21	1:B:137:ARG:HD3	2.02	0.42
1:C:206:ILE:CG2	1:C:212:LEU:HD12	2.50	0.42
1:D:7:VAL:HG12	1:D:8:ASN:N	2.33	0.42
1:A:127:GLY:HA3	1:A:189:THR:HG21	2.00	0.42
1:B:219:LEU:C	1:B:219:LEU:HD23	2.44	0.42
1:C:6:MET:SD	1:C:16:VAL:HG22	2.59	0.42
1:D:124:ILE:CD1	1:D:172:LEU:HD13	2.50	0.42
1:A:132:GLY:HA3	1:A:133:ILE:HA	1.90	0.42
1:D:12:SER:O	1:D:13:GLU:C	2.63	0.42
1:D:47:ILE:HD11	1:D:53:MET:SD	2.60	0.42
1:B:127:GLY:HA2	1:B:187:THR:O	2.19	0.42
1:C:187:THR:O	1:C:189:THR:HG22	2.19	0.42
1:E:37:THR:OG1	1:E:39:THR:HG23	2.20	0.42
1:A:8:ASN:ND2	1:A:16:VAL:CB	2.83	0.42
1:B:55:GLN:NE2	1:B:80:ARG:HG2	2.34	0.42
1:B:84:ASN:HD21	1:B:88:THR:N	2.18	0.42
1:B:126:GLU:O	1:B:186:ILE:HA	2.19	0.42
1:D:165:ALA:HB2	1:E:240:LEU:HD22	2.01	0.42
1:E:27:PRO:HA	1:E:88:THR:O	2.20	0.42
1:E:5:ILE:O	1:E:5:ILE:CG2	2.65	0.41
1:E:124:ILE:HD12	1:E:172:LEU:CD1	2.51	0.41
1:E:12:SER:O	1:E:13:GLU:C	2.64	0.41
1:B:10:LYS:HA	1:B:10:LYS:HD3	1.78	0.41
1:B:55:GLN:NE2	1:B:58:HIS:NE2	2.68	0.41
1:C:124:ILE:HD12	1:C:172:LEU:HD13	2.01	0.41
1:E:51:LEU:HD23	1:E:51:LEU:HA	1.86	0.41
1:E:202:ILE:O	1:E:206:ILE:HD12	2.20	0.41
1:A:24:TYR:CD1	1:A:87:ASN:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG22	1:A:90:LEU:HB2	2.01	0.41
1:A:136:GLU:HA	1:A:136:GLU:OE2	2.20	0.41
1:B:80:ARG:NH2	1:B:95:GLU:CD	2.78	0.41
1:B:210:TYR:O	1:B:212:LEU:HD23	2.21	0.41
1:D:93:MET:HE2	1:D:93:MET:HB3	1.87	0.41
1:A:4:MET:HG2	1:A:5:ILE:HD13	1.98	0.41
1:A:220:GLU:OE1	1:A:220:GLU:N	2.53	0.41
1:D:219:LEU:C	1:D:219:LEU:CD2	2.92	0.41
1:A:46:TYR:O	1:A:50:THR:HG22	2.21	0.41
1:A:84:ASN:N	1:A:84:ASN:HD22	2.17	0.41
1:B:80:ARG:HH22	1:B:95:GLU:CD	2.27	0.41
1:E:13:GLU:O	1:E:17:MET:HB2	2.21	0.41
1:E:100:SER:HA	1:E:103:ILE:HG13	2.03	0.41
1:C:41:VAL:HG23	1:C:42:LEU:N	2.36	0.40
1:D:136:GLU:O	1:D:136:GLU:CD	2.64	0.40
1:D:219:LEU:O	1:D:223:VAL:HG23	2.21	0.40
1:A:187:THR:CG2	1:A:202:ILE:HD13	2.51	0.40
1:B:111:MET:HG3	1:B:174:GLU:HB2	2.03	0.40
1:B:133:ILE:HD11	1:B:190:SER:CB	2.52	0.40
1:D:25:ASN:O	1:D:26:ASN:C	2.64	0.40
1:D:221:GLU:OE1	1:D:221:GLU:N	2.54	0.40
1:A:31:CYS:HB3	1:A:33:PHE:CE2	2.56	0.40
1:D:19:LEU:O	1:D:19:LEU:HD23	2.22	0.40
1:E:24:TYR:CD2	1:E:117:VAL:HG22	2.56	0.40

All (5) 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:B:24:TYR:OH	1:C:9:LYS:NZ[4_556]	1.67	0.53
1:D:131:ASN:ND2	1:E:245:LYS:O[18_655]	1.82	0.38
1:E:9:LYS:NZ	1:E:20:GLU:OE2[4_556]	1.87	0.33
1:B:5:ILE:CD1	1:C:105:GLU:OE1[4_556]	2.07	0.13
1:A:13:GLU:OE1	1:C:177:VAL:O[4_556]	2.09	0.11

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	241/252 (96%)	224 (93%)	16 (7%)	1 (0%)	30	54
1	B	240/252 (95%)	216 (90%)	23 (10%)	1 (0%)	30	54
1	C	241/252 (96%)	211 (88%)	23 (10%)	7 (3%)	3	9
1	D	238/252 (94%)	216 (91%)	20 (8%)	2 (1%)	16	37
1	E	241/252 (96%)	216 (90%)	21 (9%)	4 (2%)	7	19
All	All	1201/1260 (95%)	1083 (90%)	103 (9%)	15 (1%)	10	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	130	ALA
1	C	136	GLU
1	A	135	GLU
1	C	10	LYS
1	C	191	VAL
1	E	11	ALA
1	E	117	VAL
1	D	11	ALA
1	D	244	GLN
1	E	244	GLN
1	B	36	SER
1	C	11	ALA
1	C	132	GLY
1	E	10	LYS
1	C	73	GLY

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	205/214 (96%)	165 (80%)	40 (20%)	1	4
1	B	204/214 (95%)	152 (74%)	52 (26%)	0	2
1	C	205/214 (96%)	157 (77%)	48 (23%)	1	2
1	D	204/214 (95%)	164 (80%)	40 (20%)	1	4
1	E	205/214 (96%)	160 (78%)	45 (22%)	1	3
All	All	1023/1070 (96%)	798 (78%)	225 (22%)	1	3

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	ILE
1	A	6	MET
1	A	9	LYS
1	A	10	LYS
1	A	15	GLN
1	A	17	MET
1	A	19	LEU
1	A	26	ASN
1	A	28	VAL
1	A	36	SER
1	A	39	THR
1	A	47	ILE
1	A	50	THR
1	A	56	VAL
1	A	67	VAL
1	A	69	VAL
1	A	76	ARG
1	A	84	ASN
1	A	85	ASN
1	A	86	SER
1	A	88	THR
1	A	116	GLN
1	A	117	VAL
1	A	120	SER
1	A	121	GLU
1	A	131	ASN
1	A	136	GLU

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Mol	Chain	Res	Type
1	A	142	VAL
1	A	157	GLN
1	A	172	LEU
1	A	176	LEU
1	A	183	LEU
1	A	189	THR
1	A	191	VAL
1	A	193	ILE
1	A	202	ILE
1	A	218	LEU
1	A	223	VAL
1	A	231	LYS
1	B	5	ILE
1	B	6	MET
1	B	9	LYS
1	B	10	LYS
1	B	12	SER
1	B	13	GLU
1	B	15	GLN
1	B	16	VAL
1	B	17	MET
1	B	18	GLU
1	B	19	LEU
1	B	28	VAL
1	B	36	SER
1	B	37	THR
1	B	39	THR
1	B	41	VAL
1	B	47	ILE
1	B	48	VAL
1	B	49	GLU
1	B	56	VAL
1	B	60	ILE
1	B	67	VAL
1	B	69	VAL
1	B	71	VAL
1	B	74	LYS
1	B	76	ARG
1	B	84	ASN
1	B	86	SER
1	B	105	GLU
1	B	112	ASN

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Mol	Chain	Res	Type
1	B	117	VAL
1	B	131	ASN
1	B	135	GLU
1	B	142	VAL
1	B	152	LYS
1	B	161	SER
1	B	172	LEU
1	B	176	LEU
1	B	183	LEU
1	B	189	THR
1	B	190	SER
1	B	193	ILE
1	B	202	ILE
1	B	208	LYS
1	B	212	LEU
1	B	217	ASP
1	B	220	GLU
1	B	228	GLU
1	B	230	ILE
1	B	235	GLU
1	B	238	LYS
1	B	242	GLU
1	C	4	MET
1	C	7	VAL
1	C	10	LYS
1	C	13	GLU
1	C	14	SER
1	C	15	GLN
1	C	16	VAL
1	C	17	MET
1	C	18	GLU
1	C	19	LEU
1	C	23	ASN
1	C	26	ASN
1	C	37	THR
1	C	39	THR
1	C	45	SER
1	C	47	ILE
1	C	49	GLU
1	C	50	THR
1	C	56	VAL
1	C	67	VAL

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Mol	Chain	Res	Type
1	C	69	VAL
1	C	74	LYS
1	C	76	ARG
1	C	84	ASN
1	C	105	GLU
1	C	112	ASN
1	C	116	GLN
1	C	117	VAL
1	C	131	ASN
1	C	142	VAL
1	C	145	LYS
1	C	156	ILE
1	C	171	ILE
1	C	172	LEU
1	C	176	LEU
1	C	183	LEU
1	C	189	THR
1	C	191	VAL
1	C	193	ILE
1	C	202	ILE
1	C	216	THR
1	C	217	ASP
1	C	221	GLU
1	C	222	GLN
1	C	228	GLU
1	C	230	ILE
1	C	231	LYS
1	C	246	GLU
1	D	5	ILE
1	D	6	MET
1	D	9	LYS
1	D	10	LYS
1	D	13	GLU
1	D	15	GLN
1	D	17	MET
1	D	19	LEU
1	D	41	VAL
1	D	47	ILE
1	D	50	THR
1	D	56	VAL
1	D	60	ILE
1	D	67	VAL

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Mol	Chain	Res	Type
1	D	69	VAL
1	D	71	VAL
1	D	74	LYS
1	D	76	ARG
1	D	84	ASN
1	D	116	GLN
1	D	117	VAL
1	D	139	VAL
1	D	142	VAL
1	D	145	LYS
1	D	152	LYS
1	D	153	LYS
1	D	157	GLN
1	D	172	LEU
1	D	183	LEU
1	D	187	THR
1	D	191	VAL
1	D	202	ILE
1	D	206	ILE
1	D	213	LYS
1	D	216	THR
1	D	218	LEU
1	D	219	LEU
1	D	221	GLU
1	D	228	GLU
1	D	230	ILE
1	E	5	ILE
1	E	6	MET
1	E	8	ASN
1	E	9	LYS
1	E	10	LYS
1	E	13	GLU
1	E	15	GLN
1	E	16	VAL
1	E	17	MET
1	E	19	LEU
1	E	37	THR
1	E	39	THR
1	E	47	ILE
1	E	50	THR
1	E	56	VAL
1	E	60	ILE

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Mol	Chain	Res	Type
1	E	67	VAL
1	E	69	VAL
1	E	71	VAL
1	E	76	ARG
1	E	81	ILE
1	E	84	ASN
1	E	86	SER
1	E	99	SER
1	E	105	GLU
1	E	116	GLN
1	E	117	VAL
1	E	121	GLU
1	E	131	ASN
1	E	133	ILE
1	E	142	VAL
1	E	150	LYS
1	E	172	LEU
1	E	176	LEU
1	E	183	LEU
1	E	191	VAL
1	E	193	ILE
1	E	202	ILE
1	E	218	LEU
1	E	222	GLN
1	E	224	LYS
1	E	228	GLU
1	E	230	ILE
1	E	231	LYS
1	E	242	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	55	GLN
1	A	58	HIS
1	A	84	ASN
1	A	112	ASN
1	A	116	GLN
1	A	131	ASN
1	A	157	GLN
1	A	211	ASN

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	55	GLN
1	B	84	ASN
1	B	108	ASN
1	B	131	ASN
1	B	157	GLN
1	B	222	GLN
1	B	229	GLN
1	C	26	ASN
1	C	58	HIS
1	C	63	HIS
1	C	84	ASN
1	C	108	ASN
1	C	112	ASN
1	C	157	GLN
1	C	211	ASN
1	C	222	GLN
1	D	15	GLN
1	D	55	GLN
1	D	58	HIS
1	D	84	ASN
1	D	112	ASN
1	D	211	ASN
1	D	222	GLN
1	E	8	ASN
1	E	15	GLN
1	E	58	HIS
1	E	84	ASN
1	E	85	ASN
1	E	87	ASN
1	E	102	HIS
1	E	108	ASN
1	E	112	ASN
1	E	131	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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(Å ²)	Q<0.9
1	A	243/252 (96%)	-0.19	6 (2%) 58 55	22, 40, 73, 93	0
1	B	242/252 (96%)	-0.17	2 (0%) 82 81	32, 43, 63, 92	0
1	C	243/252 (96%)	-0.09	3 (1%) 76 75	35, 48, 73, 88	0
1	D	242/252 (96%)	-0.15	7 (2%) 53 50	20, 48, 78, 95	0
1	E	243/252 (96%)	-0.14	7 (2%) 53 50	33, 47, 73, 85	0
All	All	1213/1260 (96%)	-0.15	25 (2%) 63 61	20, 45, 73, 95	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	VAL	5.4
1	B	6	MET	4.3
1	C	136	GLU	3.4
1	A	19	LEU	3.2
1	E	7	VAL	3.1
1	A	13	GLU	2.9
1	A	8	ASN	2.9
1	D	134	PRO	2.8
1	D	4	MET	2.7
1	E	8	ASN	2.7
1	D	132	GLY	2.6
1	E	6	MET	2.5
1	C	7	VAL	2.4
1	D	16	VAL	2.4
1	E	133	ILE	2.4
1	E	4	MET	2.3
1	D	6	MET	2.3
1	E	233	ILE	2.3
1	D	13	GLU	2.2
1	E	19	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	6	MET	2.2
1	A	7	VAL	2.2
1	D	19	LEU	2.1
1	A	4	MET	2.1
1	C	11	ALA	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.