



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:32 PM UTC

PDB ID : 2AYI / pdb_00002ayi
Title : Wild-type AmpT from *Thermus thermophilus*
Authors : Odintsov, S.G.; Sabala, I.; Bourenkov, G.; Rybin, V.; Bochtler, M.
Deposited on : 2005-09-07
Resolution : 3.70 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

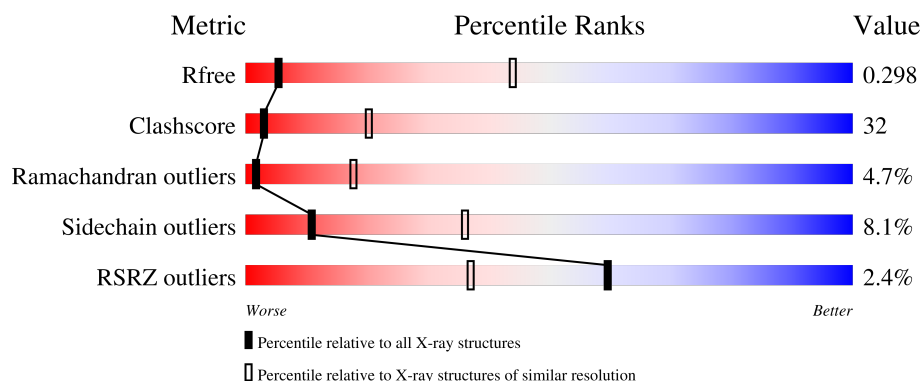
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	408	% 52% 37% 8% ..
1	B	408	4% 54% 35% 8% ..
1	C	408	54% 35% 8% .
1	D	408	5% 51% 37% 8% ..
1	E	408	% 54% 35% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15475 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 Aminopeptidase T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3093	1963	563	562	5			
1	B	397	Total	C	N	O	S	0	0	0
			3093	1963	563	562	5			
1	C	397	Total	C	N	O	S	0	0	0
			3093	1963	563	562	5			
1	D	397	Total	C	N	O	S	0	0	0
			3093	1963	563	562	5			
1	E	397	Total	C	N	O	S	0	0	0
			3093	1963	563	562	5			

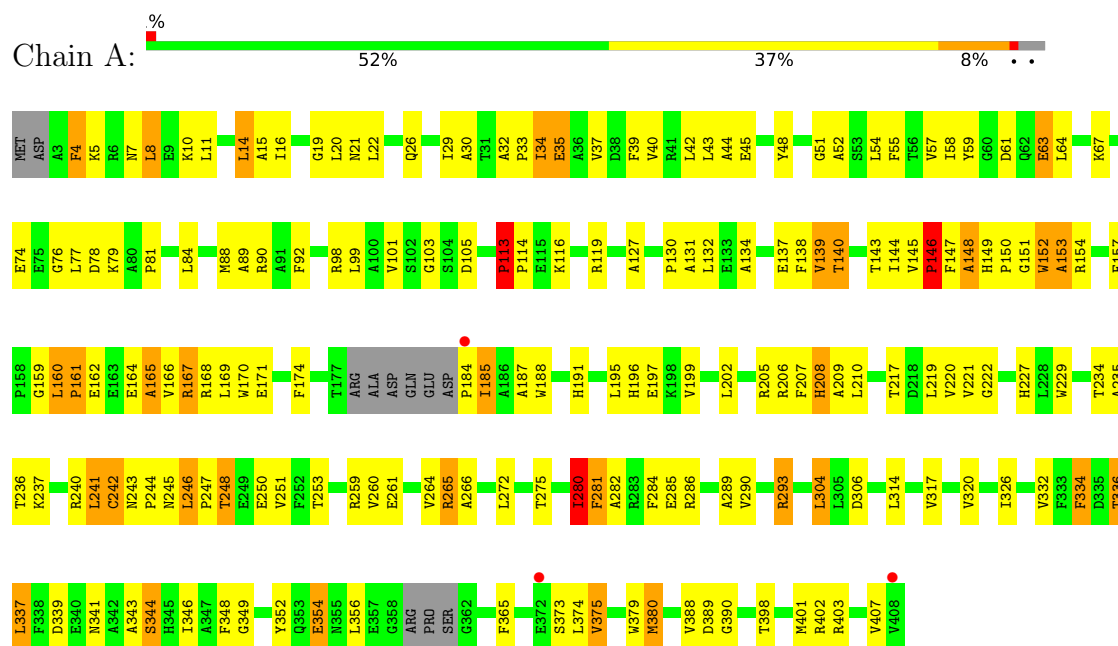
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

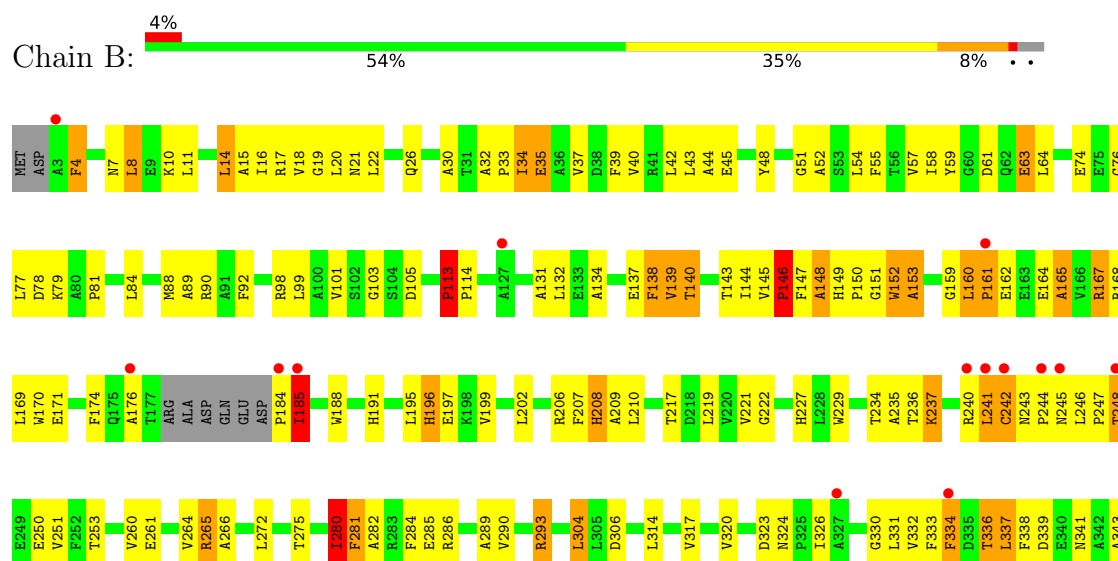
3 Residue-property plots

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: Aminopeptidase T



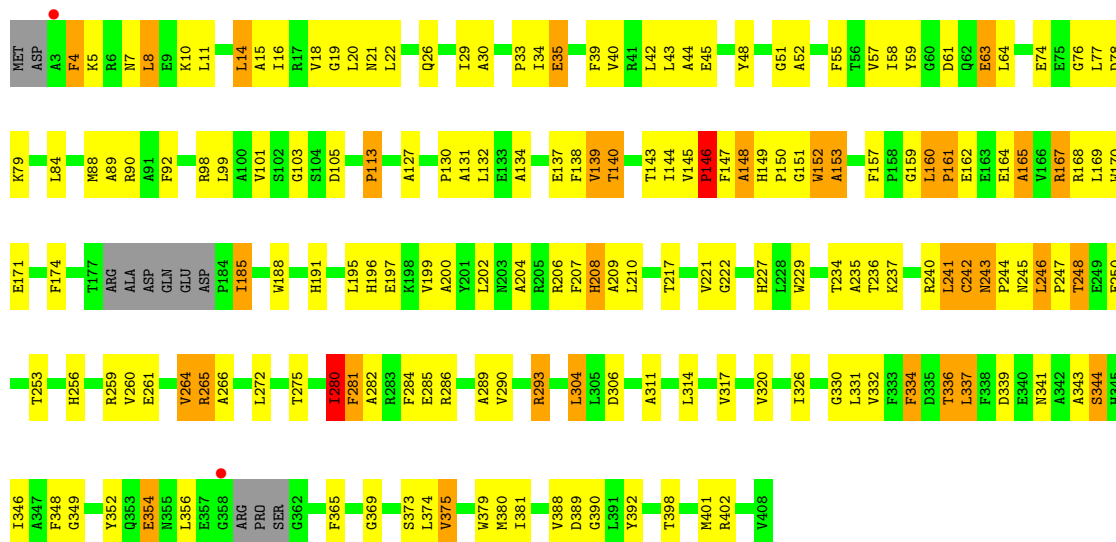
• Molecule 1: Aminopeptidase T





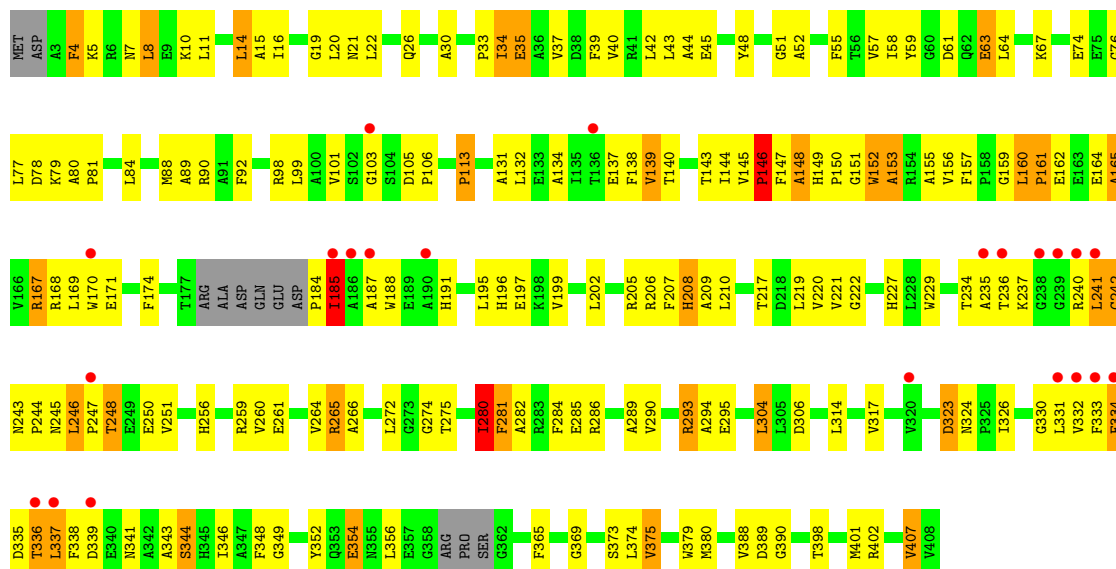
• Molecule 1: Aminopeptidase T

Chain C: 54% 35% 8%



• Molecule 1: Aminopeptidase T

Chain D: 51% 37% 8%



• Molecule 1: Aminopeptidase T

Chain E: 54% 35% 8%



S344	H345	I346	A347	F348	G349		Y352	Q353	E354	N355	L356	E357	G358	ARG	PRO	SER	G362		F365		S373	L374	V375		W379	M380		V388	D389	G390	L391	Y392		T398		M401	R402	R403		V408																			
P244	N245	L246	P247	T248	E249	E250	V251		R259	V260	E261		V264	R265	A266		L272		T275		L280	F281	A282	R283	F284	E285	R286		A289	V290		R293		L304	L305	D306		L314		V317		V320		D323	N324	P325	I326		F333	F334	D335	T336	L337	F338	D339	E340	N341	A342	A343
E164	A165	V166	R167	R168	L169	W170	E171		F174	Q175	A176	T177	ARG	ALA	ASP	GLN	GLU	ASP	P184	I185		W188		H191		L195	H196	E197	K198	V199		L202		R206	F207	H208	A209	L210		T217	D218	L219	V220	V221	G222		H227	L228	W229		T234	A235	T236	K237		R240	L241	C242	N243
E74	E75	G76	L77	D78	K79	A80	P81		L84		M88		F92		R98	L99	A100	V101	S102	G103	S104	D105		P113	P114		A127		P130	A131	L132	E133	A134		E137	F138	V139	T140		T143	I144	V145	P146	F147	A148	H149	P150	G151	W152	A153	R154		F157	P158	G159	L160	P161	E162	E163
MET	ASP	A3	F4	K5	R6	N7	L8	E9	K10	L11		L14	A15	I16	R17	V18	G19	L20	N21	L22		Q26		A30	T31	A32	P33	I34	E35	A36	V37	D38	F39	V40	R41	L42	L43	A44	E45		Y48		G51	A52	S53	L54	F55	T56	V57	I58	Y59	O60	D61	Q62	E63	L64		K67	

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	246.47Å 246.47Å 51.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.71	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.70) 97.7 (20.00-3.71)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.84 (at 3.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.308 , 0.321 0.293 , 0.298	Depositor DCC
R_{free} test set	1629 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	131.5	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15475	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.69	0/3161	1.05	18/4277 (0.4%)
1	B	0.71	0/3161	1.05	16/4277 (0.4%)
1	C	0.69	1/3161 (0.0%)	1.04	17/4277 (0.4%)
1	D	0.72	0/3161	1.05	19/4277 (0.4%)
1	E	0.72	1/3161 (0.0%)	1.04	17/4277 (0.4%)
All	All	0.71	2/15805 (0.0%)	1.05	87/21385 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	264	VAL	CA-CB	-5.21	1.48	1.54
1	E	152	TRP	CA-C	-5.04	1.48	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	243	ASN	CA-C-N	7.28	126.54	118.97
1	D	243	ASN	C-N-CA	7.28	126.54	118.97
1	E	162	GLU	N-CA-C	-6.84	103.28	111.69
1	C	243	ASN	CA-C-N	6.78	126.02	118.97
1	C	243	ASN	C-N-CA	6.78	126.02	118.97
1	B	162	GLU	N-CA-C	-6.66	103.50	111.69
1	C	165	ALA	N-CA-C	-6.66	103.95	111.14
1	A	153	ALA	N-CA-C	-6.63	104.29	112.38
1	D	162	GLU	N-CA-C	-6.61	104.16	111.36
1	B	153	ALA	N-CA-C	-6.60	104.33	112.38
1	A	243	ASN	CA-C-N	6.59	125.83	118.97
1	A	243	ASN	C-N-CA	6.59	125.83	118.97
1	D	153	ALA	N-CA-C	-6.56	104.38	112.38
1	A	162	GLU	N-CA-C	-6.50	104.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	PRO	CA-C-N	6.48	127.94	119.84
1	D	113	PRO	C-N-CA	6.48	127.94	119.84
1	A	113	PRO	CA-C-N	6.39	127.83	119.84
1	A	113	PRO	C-N-CA	6.39	127.83	119.84
1	C	113	PRO	CA-C-N	6.36	127.79	119.84
1	C	113	PRO	C-N-CA	6.36	127.79	119.84
1	E	139	VAL	N-CA-C	-6.28	106.81	111.90
1	A	165	ALA	N-CA-C	-6.24	104.40	111.14
1	C	153	ALA	N-CA-C	-6.17	104.85	112.38
1	B	165	ALA	N-CA-C	-6.08	104.57	111.14
1	E	243	ASN	CA-C-N	6.05	125.27	118.97
1	E	243	ASN	C-N-CA	6.05	125.27	118.97
1	B	243	ASN	CA-C-N	6.04	125.25	118.97
1	B	243	ASN	C-N-CA	6.04	125.25	118.97
1	C	162	GLU	N-CA-C	-6.04	104.77	111.36
1	E	153	ALA	N-CA-C	-6.03	105.02	112.38
1	B	113	PRO	CA-C-N	6.03	127.38	119.84
1	B	113	PRO	C-N-CA	6.03	127.38	119.84
1	D	165	ALA	N-CA-C	-6.01	104.65	111.14
1	A	139	VAL	N-CA-C	-5.99	107.05	111.90
1	E	113	PRO	CA-C-N	5.94	127.27	119.84
1	E	113	PRO	C-N-CA	5.94	127.27	119.84
1	D	139	VAL	N-CA-C	-5.93	107.10	111.90
1	E	259	ARG	N-CA-C	5.91	117.53	110.44
1	D	259	ARG	N-CA-C	5.90	117.62	109.54
1	E	165	ALA	N-CA-C	-5.85	104.82	111.14
1	D	208	HIS	N-CA-C	-5.72	106.65	113.97
1	C	375	VAL	N-CA-C	5.70	117.80	108.97
1	B	375	VAL	N-CA-C	5.69	117.78	108.97
1	E	208	HIS	N-CA-C	-5.63	106.76	113.97
1	E	375	VAL	N-CA-C	5.61	117.66	108.97
1	D	375	VAL	N-CA-C	5.61	117.66	108.97
1	A	259	ARG	N-CA-C	5.60	117.21	109.54
1	A	208	HIS	N-CA-C	-5.59	106.82	113.97
1	C	259	ARG	N-CA-C	5.55	117.15	109.54
1	B	21	ASN	N-CA-C	-5.53	104.27	111.74
1	B	208	HIS	N-CA-C	-5.52	106.91	113.97
1	A	21	ASN	N-CA-C	-5.48	104.34	111.74
1	C	21	ASN	N-CA-C	-5.47	104.35	111.74
1	E	21	ASN	N-CA-C	-5.46	104.37	111.74
1	C	208	HIS	N-CA-C	-5.46	106.98	113.97
1	B	139	VAL	N-CA-C	-5.43	107.50	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	VAL	N-CA-C	5.42	117.37	108.97
1	D	187	ALA	N-CA-C	-5.41	105.82	112.90
1	E	4	PHE	N-CA-C	-5.37	106.86	113.41
1	B	323	ASP	N-CA-C	-5.36	106.05	112.59
1	B	191	HIS	N-CA-C	-5.35	106.81	113.55
1	A	187	ALA	N-CA-C	-5.34	105.91	112.90
1	D	4	PHE	N-CA-C	-5.31	106.93	113.41
1	C	139	VAL	N-CA-C	-5.31	107.60	111.90
1	B	250	GLU	N-CA-C	5.30	118.28	110.59
1	B	185	ILE	N-CA-C	-5.30	104.88	112.35
1	C	5	LYS	N-CA-C	-5.30	105.61	111.71
1	A	4	PHE	N-CA-C	-5.29	107.00	113.50
1	D	191	HIS	N-CA-C	-5.27	106.91	113.55
1	E	191	HIS	N-CA-C	-5.23	106.96	113.55
1	E	323	ASP	N-CA-C	-5.22	106.22	112.59
1	C	191	HIS	N-CA-C	-5.20	107.00	113.55
1	A	5	LYS	N-CA-C	-5.18	105.75	111.71
1	D	21	ASN	N-CA-C	-5.18	104.75	111.74
1	D	5	LYS	N-CA-C	-5.15	105.79	111.71
1	D	250	GLU	N-CA-C	5.13	118.03	110.59
1	E	5	LYS	N-CA-C	-5.13	105.81	111.71
1	A	250	GLU	N-CA-C	5.11	117.99	110.59
1	C	250	GLU	N-CA-C	5.10	117.98	110.59
1	C	4	PHE	N-CA-C	-5.09	107.20	113.41
1	A	191	HIS	N-CA-C	-5.08	107.15	113.55
1	D	407	VAL	CA-C-O	5.05	123.53	118.98
1	E	250	GLU	N-CA-C	5.03	117.88	110.59
1	D	323	ASP	N-CA-C	-5.02	106.46	112.59
1	B	4	PHE	N-CA-C	-5.02	107.32	113.50
1	C	381	ILE	N-CA-C	-5.02	108.94	113.71
1	A	166	VAL	N-CA-C	-5.01	105.61	110.42

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	3093	0	3067	197	0
1	B	3093	0	3067	206	0
1	C	3093	0	3067	191	0
1	D	3093	0	3067	227	1
1	E	3093	0	3067	199	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
All	All	15475	0	15335	979	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 32.

All (979) 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:206:ARG:HH21	1:D:293:ARG:NE	1.40	1.19
1:D:152:TRP:NE1	1:D:333:PHE:O	1.81	1.14
1:D:156:VAL:HG13	1:D:331:LEU:HB3	1.20	1.14
1:C:206:ARG:NH2	1:D:293:ARG:NE	1.96	1.11
1:A:105:ASP:HB2	1:A:151:GLY:HA3	1.33	1.10
1:C:105:ASP:HB2	1:C:151:GLY:HA3	1.34	1.10
1:D:105:ASP:HB2	1:D:151:GLY:HA3	1.35	1.06
1:D:184:PRO:HD2	1:D:185:ILE:HD12	1.35	1.04
1:B:105:ASP:HB2	1:B:151:GLY:HA3	1.37	1.03
1:D:152:TRP:CZ2	1:D:333:PHE:HB3	1.94	1.01
1:B:138:PHE:HB3	1:B:236:THR:HA	1.41	1.01
1:E:105:ASP:HB2	1:E:151:GLY:HA3	1.39	1.00
1:D:14:LEU:HD21	1:D:246:LEU:HD11	1.43	1.00
1:B:17:ARG:HB3	1:B:185:ILE:HG21	1.44	0.96
1:D:106:PRO:O	1:D:274:GLY:HA2	1.63	0.96
1:A:164:GLU:HA	1:A:167:ARG:HB2	1.48	0.95
1:B:140:THR:C	1:B:236:THR:HG21	1.92	0.94
1:D:164:GLU:HA	1:D:167:ARG:HB2	1.49	0.94
1:B:164:GLU:HA	1:B:167:ARG:HB2	1.49	0.94
1:C:164:GLU:HA	1:C:167:ARG:HB2	1.49	0.93
1:B:140:THR:O	1:B:236:THR:HG21	1.67	0.93
1:B:17:ARG:HB3	1:B:185:ILE:CG2	2.00	0.91
1:C:206:ARG:HH21	1:D:293:ARG:HE	1.19	0.90
1:E:164:GLU:HA	1:E:167:ARG:HB2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TRP:HE3	1:B:169:LEU:HD21	1.39	0.88
1:A:152:TRP:HE3	1:A:169:LEU:HD21	1.38	0.86
1:D:152:TRP:HE3	1:D:169:LEU:HD21	1.38	0.86
1:D:184:PRO:HD2	1:D:185:ILE:CD1	2.04	0.86
1:E:147:PHE:CZ	1:E:170:TRP:HB2	2.11	0.85
1:B:147:PHE:CZ	1:B:170:TRP:HB2	2.12	0.85
1:C:147:PHE:CZ	1:C:170:TRP:HB2	2.12	0.84
1:A:147:PHE:CZ	1:A:170:TRP:HB2	2.12	0.84
1:B:143:THR:HG22	1:B:144:ILE:H	1.41	0.84
1:E:152:TRP:HE3	1:E:169:LEU:HD21	1.40	0.84
1:D:143:THR:HG22	1:D:144:ILE:H	1.42	0.84
1:C:143:THR:HG22	1:C:144:ILE:N	1.91	0.84
1:C:143:THR:HG22	1:C:144:ILE:H	1.43	0.84
1:D:147:PHE:CZ	1:D:170:TRP:HB2	2.13	0.83
1:D:156:VAL:HG13	1:D:331:LEU:CB	2.07	0.83
1:C:152:TRP:HE3	1:C:169:LEU:HD21	1.41	0.83
1:B:143:THR:HG22	1:B:144:ILE:N	1.92	0.83
1:E:143:THR:HG22	1:E:144:ILE:N	1.93	0.83
1:E:143:THR:HG22	1:E:144:ILE:H	1.45	0.82
1:A:143:THR:HG22	1:A:144:ILE:N	1.94	0.82
1:A:143:THR:HG22	1:A:144:ILE:H	1.45	0.82
1:B:138:PHE:CB	1:B:236:THR:HA	2.11	0.80
1:D:156:VAL:HG11	1:D:331:LEU:HD13	1.64	0.80
1:B:134:ALA:O	1:B:139:VAL:HG22	1.83	0.79
1:D:143:THR:HG22	1:D:144:ILE:N	1.94	0.79
1:B:144:ILE:O	1:B:246:LEU:HD23	1.82	0.79
1:C:185:ILE:HD12	1:C:185:ILE:H	1.47	0.79
1:E:61:ASP:HB3	1:E:64:LEU:HD12	1.65	0.78
1:D:14:LEU:C	1:D:14:LEU:HD23	2.08	0.78
1:D:61:ASP:HB3	1:D:64:LEU:HD12	1.66	0.77
1:D:134:ALA:O	1:D:139:VAL:HG22	1.85	0.77
1:E:134:ALA:O	1:E:139:VAL:HG22	1.84	0.77
1:C:14:LEU:C	1:C:14:LEU:HD23	2.11	0.76
1:B:139:VAL:HA	1:B:237:LYS:HB2	1.65	0.76
1:C:206:ARG:NH2	1:D:293:ARG:CZ	2.48	0.76
1:D:161:PRO:HB2	1:D:164:GLU:HB3	1.67	0.76
1:E:161:PRO:HB2	1:E:164:GLU:HB3	1.67	0.76
1:A:293:ARG:NE	1:E:206:ARG:HH21	1.83	0.76
1:A:61:ASP:HB3	1:A:64:LEU:HD12	1.66	0.76
1:C:293:ARG:NH1	1:C:293:ARG:HB3	2.01	0.76
1:A:261:GLU:HG2	1:A:286:ARG:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PRO:HB2	1:B:164:GLU:HB3	1.67	0.76
1:C:61:ASP:HB3	1:C:64:LEU:HD12	1.66	0.76
1:D:247:PRO:HD2	1:D:337:LEU:HD11	1.68	0.75
1:A:161:PRO:HB2	1:A:164:GLU:HB3	1.68	0.75
1:D:152:TRP:CE3	1:D:169:LEU:HD21	2.22	0.75
1:C:134:ALA:O	1:C:139:VAL:HG22	1.86	0.75
1:C:161:PRO:HB2	1:C:164:GLU:HB3	1.69	0.74
1:B:61:ASP:HB3	1:B:64:LEU:HD12	1.68	0.74
1:B:14:LEU:HD23	1:B:14:LEU:C	2.13	0.74
1:A:134:ALA:O	1:A:139:VAL:HG22	1.87	0.74
1:B:18:VAL:HG23	1:B:185:ILE:HG23	1.70	0.74
1:B:293:ARG:HB3	1:B:293:ARG:NH1	2.01	0.74
1:A:293:ARG:NH1	1:A:293:ARG:HB3	2.03	0.73
1:C:105:ASP:CB	1:C:151:GLY:HA3	2.17	0.73
1:B:152:TRP:CE3	1:B:169:LEU:HD21	2.22	0.73
1:E:293:ARG:HB3	1:E:293:ARG:NH1	2.04	0.73
1:E:152:TRP:CE3	1:E:169:LEU:HD21	2.23	0.73
1:B:261:GLU:HG2	1:B:286:ARG:H	1.54	0.73
1:D:293:ARG:HB3	1:D:293:ARG:NH1	2.04	0.73
1:E:14:LEU:C	1:E:14:LEU:HD23	2.14	0.73
1:A:185:ILE:H	1:A:185:ILE:HD12	1.53	0.73
1:B:185:ILE:HD12	1:B:185:ILE:H	1.53	0.73
1:E:261:GLU:HG2	1:E:286:ARG:H	1.52	0.73
1:A:14:LEU:C	1:A:14:LEU:HD23	2.14	0.72
1:A:152:TRP:CE3	1:A:169:LEU:HD21	2.22	0.72
1:C:261:GLU:HG2	1:C:286:ARG:H	1.54	0.72
1:A:105:ASP:CB	1:A:151:GLY:HA3	2.18	0.72
1:B:266:ALA:HB2	1:B:280:ILE:HG23	1.72	0.72
1:E:241:LEU:HD12	1:E:241:LEU:H	1.55	0.72
1:C:247:PRO:HD2	1:C:337:LEU:HD11	1.70	0.72
1:E:147:PHE:HZ	1:E:170:TRP:HB2	1.53	0.71
1:C:314:LEU:HD22	1:C:346:ILE:HG13	1.72	0.71
1:A:314:LEU:HD22	1:A:346:ILE:HG13	1.72	0.71
1:B:15:ALA:CB	1:B:145:VAL:HG21	2.21	0.71
1:B:138:PHE:HB3	1:B:236:THR:CA	2.20	0.71
1:C:206:ARG:HH21	1:D:293:ARG:CD	2.04	0.71
1:C:339:ASP:HB3	1:C:380:MET:HE3	1.72	0.71
1:D:261:GLU:HG2	1:D:286:ARG:H	1.56	0.70
1:A:40:VAL:HG21	1:A:59:TYR:HE1	1.56	0.70
1:A:247:PRO:HD2	1:A:337:LEU:HD11	1.73	0.70
1:C:147:PHE:HZ	1:C:170:TRP:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:THR:HA	1:D:341:ASN:OD1	1.91	0.70
1:A:266:ALA:HB2	1:A:280:ILE:HG23	1.73	0.70
1:D:105:ASP:CB	1:D:151:GLY:HA3	2.19	0.70
1:B:170:TRP:HD1	1:B:171:GLU:N	1.90	0.70
1:B:241:LEU:HD12	1:B:241:LEU:H	1.56	0.70
1:A:147:PHE:HZ	1:A:170:TRP:HB2	1.56	0.70
1:C:266:ALA:HB2	1:C:280:ILE:HG23	1.74	0.70
1:C:248:THR:HA	1:C:341:ASN:OD1	1.92	0.69
1:E:15:ALA:CB	1:E:145:VAL:HG21	2.21	0.69
1:A:241:LEU:HD12	1:A:241:LEU:H	1.57	0.69
1:B:339:ASP:HB3	1:B:380:MET:HE3	1.74	0.69
1:D:106:PRO:HG3	1:D:334:PHE:CG	2.28	0.69
1:C:209:ALA:HB2	1:C:222:GLY:HA2	1.75	0.69
1:C:152:TRP:CE3	1:C:169:LEU:HD21	2.25	0.69
1:C:170:TRP:HD1	1:C:171:GLU:N	1.91	0.69
1:E:40:VAL:HG21	1:E:59:TYR:HE1	1.58	0.69
1:D:314:LEU:HD22	1:D:346:ILE:HG13	1.74	0.69
1:A:339:ASP:HB3	1:A:380:MET:HE3	1.74	0.69
1:D:15:ALA:CB	1:D:145:VAL:HG21	2.23	0.69
1:E:314:LEU:HD22	1:E:346:ILE:HG13	1.75	0.68
1:A:349:GLY:HA3	1:A:375:VAL:O	1.92	0.68
1:D:144:ILE:HG22	1:D:337:LEU:HD22	1.76	0.68
1:D:339:ASP:HB3	1:D:380:MET:HE3	1.74	0.68
1:E:339:ASP:HB3	1:E:380:MET:HE3	1.73	0.68
1:B:314:LEU:HD22	1:B:346:ILE:HG13	1.74	0.68
1:D:147:PHE:HZ	1:D:170:TRP:HB2	1.57	0.68
1:C:40:VAL:HG21	1:C:59:TYR:HE1	1.59	0.68
1:C:143:THR:CG2	1:C:246:LEU:CD2	2.71	0.68
1:D:40:VAL:HG21	1:D:59:TYR:HE1	1.56	0.68
1:D:156:VAL:CG1	1:D:331:LEU:HB3	2.11	0.68
1:B:349:GLY:HA3	1:B:375:VAL:O	1.93	0.68
1:B:105:ASP:CB	1:B:151:GLY:HA3	2.20	0.68
1:C:15:ALA:CB	1:C:145:VAL:HG21	2.23	0.68
1:D:170:TRP:HD1	1:D:171:GLU:N	1.91	0.68
1:A:293:ARG:NE	1:E:206:ARG:NH2	2.42	0.68
1:A:352:TYR:HB3	1:A:354:GLU:HG3	1.76	0.68
1:B:147:PHE:HZ	1:B:170:TRP:HB2	1.55	0.68
1:D:209:ALA:HB2	1:D:222:GLY:HA2	1.75	0.68
1:E:352:TYR:HB3	1:E:354:GLU:HG3	1.76	0.68
1:A:15:ALA:CB	1:A:145:VAL:HG21	2.23	0.67
1:B:209:ALA:HB2	1:B:222:GLY:HA2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ALA:CB	1:C:222:GLY:HA2	2.24	0.67
1:B:40:VAL:HG21	1:B:59:TYR:HE1	1.59	0.67
1:E:266:ALA:HB2	1:E:280:ILE:HG23	1.75	0.67
1:E:43:LEU:HD13	1:E:99:LEU:HD21	1.77	0.67
1:E:247:PRO:HD2	1:E:337:LEU:HD11	1.76	0.67
1:E:221:VAL:HA	1:E:260:VAL:HG13	1.77	0.67
1:C:43:LEU:HD13	1:C:99:LEU:HD21	1.76	0.67
1:A:170:TRP:HD1	1:A:171:GLU:N	1.92	0.67
1:C:221:VAL:HA	1:C:260:VAL:HG13	1.77	0.67
1:E:170:TRP:HD1	1:E:171:GLU:N	1.92	0.67
1:B:209:ALA:CB	1:B:222:GLY:HA2	2.25	0.67
1:B:143:THR:CG2	1:B:144:ILE:H	2.08	0.67
1:D:106:PRO:HG3	1:D:334:PHE:CD1	2.29	0.67
1:D:209:ALA:CB	1:D:222:GLY:HA2	2.24	0.67
1:E:105:ASP:CB	1:E:151:GLY:HA3	2.22	0.67
1:B:43:LEU:HD13	1:B:99:LEU:HD21	1.76	0.66
1:D:43:LEU:HD13	1:D:99:LEU:HD21	1.76	0.66
1:E:209:ALA:HB2	1:E:222:GLY:HA2	1.77	0.66
1:B:138:PHE:O	1:B:237:LYS:N	2.28	0.66
1:A:248:THR:HA	1:A:341:ASN:OD1	1.96	0.66
1:D:352:TYR:HB3	1:D:354:GLU:HG3	1.77	0.66
1:C:349:GLY:HA3	1:C:375:VAL:O	1.93	0.66
1:B:18:VAL:HG11	1:B:188:TRP:HB3	1.77	0.66
1:B:247:PRO:HD2	1:B:337:LEU:HD11	1.78	0.66
1:C:352:TYR:HB3	1:C:354:GLU:HG3	1.78	0.66
1:E:161:PRO:CB	1:E:164:GLU:HB3	2.26	0.66
1:D:241:LEU:H	1:D:241:LEU:HD12	1.59	0.66
1:A:43:LEU:HD13	1:A:99:LEU:HD21	1.76	0.65
1:C:241:LEU:HD12	1:C:241:LEU:H	1.60	0.65
1:E:349:GLY:HA3	1:E:375:VAL:O	1.95	0.65
1:A:209:ALA:HB2	1:A:222:GLY:HA2	1.78	0.65
1:B:352:TYR:HB3	1:B:354:GLU:HG3	1.79	0.65
1:D:349:GLY:HA3	1:D:375:VAL:O	1.96	0.65
1:B:138:PHE:C	1:B:236:THR:HG23	2.21	0.65
1:A:265:ARG:NH1	1:E:392:TYR:CD2	2.65	0.65
1:D:143:THR:CG2	1:D:144:ILE:H	2.09	0.65
1:B:161:PRO:CB	1:B:164:GLU:HB3	2.27	0.65
1:C:147:PHE:O	1:C:148:ALA:O	2.15	0.65
1:D:156:VAL:CG1	1:D:331:LEU:HD13	2.27	0.65
1:D:147:PHE:O	1:D:148:ALA:O	2.15	0.64
1:A:209:ALA:CB	1:A:222:GLY:HA2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:O	1:B:148:ALA:O	2.14	0.64
1:D:266:ALA:HB2	1:D:280:ILE:HG23	1.78	0.64
1:A:221:VAL:HA	1:A:260:VAL:HG13	1.80	0.64
1:E:248:THR:HA	1:E:341:ASN:OD1	1.98	0.64
1:E:149:HIS:C	1:E:151:GLY:H	2.06	0.64
1:E:209:ALA:CB	1:E:222:GLY:HA2	2.27	0.64
1:C:143:THR:CG2	1:C:144:ILE:N	2.61	0.64
1:C:143:THR:CG2	1:C:144:ILE:H	2.10	0.64
1:E:185:ILE:HD12	1:E:185:ILE:H	1.62	0.64
1:A:161:PRO:CB	1:A:164:GLU:HB3	2.28	0.63
1:A:147:PHE:O	1:A:148:ALA:O	2.16	0.63
1:D:161:PRO:CB	1:D:164:GLU:HB3	2.28	0.63
1:A:92:PHE:CZ	1:A:98:ARG:HG3	2.34	0.63
1:E:147:PHE:O	1:E:148:ALA:O	2.16	0.63
1:C:161:PRO:CB	1:C:164:GLU:HB3	2.29	0.62
1:D:221:VAL:HA	1:D:260:VAL:HG13	1.81	0.62
1:E:40:VAL:CG1	1:E:57:VAL:HG11	2.30	0.62
1:A:143:THR:CG2	1:A:144:ILE:N	2.63	0.61
1:A:207:PHE:CE2	1:A:390:GLY:HA3	2.35	0.61
1:B:15:ALA:HB1	1:B:145:VAL:HG21	1.81	0.61
1:B:138:PHE:CE2	1:B:234:THR:HG21	2.35	0.61
1:B:248:THR:HA	1:B:341:ASN:OD1	2.00	0.61
1:A:285:GLU:O	1:A:286:ARG:HG2	2.01	0.61
1:B:40:VAL:CG1	1:B:57:VAL:HG11	2.31	0.61
1:B:149:HIS:C	1:B:151:GLY:H	2.07	0.61
1:E:58:ILE:CD1	1:E:84:LEU:HD11	2.30	0.61
1:E:143:THR:CG2	1:E:144:ILE:H	2.11	0.61
1:D:15:ALA:HB1	1:D:145:VAL:HG21	1.83	0.61
1:A:143:THR:CG2	1:A:144:ILE:H	2.11	0.61
1:C:40:VAL:CG1	1:C:57:VAL:HG11	2.31	0.61
1:C:153:ALA:HB1	1:C:165:ALA:CB	2.31	0.61
1:E:18:VAL:CG2	1:E:185:ILE:HG23	2.30	0.61
1:B:221:VAL:HA	1:B:260:VAL:HG13	1.81	0.61
1:D:207:PHE:CE2	1:D:390:GLY:HA3	2.36	0.61
1:C:58:ILE:CD1	1:C:84:LEU:HD11	2.31	0.61
1:A:15:ALA:HB1	1:A:145:VAL:HG21	1.82	0.60
1:A:40:VAL:CG1	1:A:57:VAL:HG11	2.31	0.60
1:B:58:ILE:CD1	1:B:84:LEU:HD11	2.30	0.60
1:D:242:CYS:O	1:D:244:PRO:HD3	2.01	0.60
1:A:153:ALA:HB1	1:A:165:ALA:CB	2.32	0.60
1:B:139:VAL:C	1:B:236:THR:HG22	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:VAL:CG1	1:D:57:VAL:HG11	2.32	0.60
1:B:14:LEU:HD11	1:B:188:TRP:NE1	2.17	0.60
1:D:67:LYS:HD3	1:E:45:GLU:HB2	1.82	0.60
1:C:14:LEU:HD21	1:C:246:LEU:HD11	1.84	0.60
1:D:149:HIS:C	1:D:151:GLY:H	2.10	0.60
1:B:176:ALA:CB	1:B:338:PHE:CZ	2.84	0.60
1:C:242:CYS:O	1:C:244:PRO:HD3	2.01	0.60
1:D:156:VAL:HG22	1:D:332:VAL:O	2.02	0.60
1:A:149:HIS:C	1:A:151:GLY:H	2.09	0.60
1:E:15:ALA:HB2	1:E:145:VAL:HG21	1.83	0.60
1:A:260:VAL:O	1:A:284:PHE:HB3	2.01	0.59
1:E:285:GLU:O	1:E:286:ARG:HG2	2.01	0.59
1:B:236:THR:HB	1:B:240:ARG:HB3	1.85	0.59
1:E:92:PHE:CZ	1:E:98:ARG:HG3	2.37	0.59
1:A:242:CYS:O	1:A:244:PRO:HD3	2.01	0.59
1:B:92:PHE:CZ	1:B:98:ARG:HG3	2.37	0.59
1:C:15:ALA:HB1	1:C:145:VAL:HG21	1.83	0.59
1:D:153:ALA:HB1	1:D:165:ALA:CB	2.32	0.59
1:D:40:VAL:HG21	1:D:59:TYR:CE1	2.38	0.59
1:C:92:PHE:CZ	1:C:98:ARG:HG3	2.38	0.59
1:C:392:TYR:CD2	1:D:265:ARG:NH1	2.71	0.59
1:E:207:PHE:CE2	1:E:390:GLY:HA3	2.37	0.59
1:B:14:LEU:HD11	1:B:188:TRP:CD1	2.38	0.59
1:C:260:VAL:O	1:C:284:PHE:HB3	2.03	0.59
1:E:236:THR:HB	1:E:240:ARG:HB3	1.85	0.59
1:B:293:ARG:HB3	1:B:293:ARG:HH11	1.67	0.59
1:C:149:HIS:C	1:C:151:GLY:H	2.11	0.59
1:D:152:TRP:CE2	1:D:333:PHE:O	2.55	0.59
1:D:184:PRO:CD	1:D:185:ILE:HD12	2.20	0.59
1:A:143:THR:CG2	1:A:246:LEU:CD2	2.81	0.58
1:A:160:LEU:HB2	1:A:161:PRO:HD3	1.85	0.58
1:D:92:PHE:CZ	1:D:98:ARG:HG3	2.37	0.58
1:D:106:PRO:HB3	1:D:334:PHE:HB3	1.85	0.58
1:D:260:VAL:O	1:D:284:PHE:HB3	2.03	0.58
1:E:15:ALA:HB1	1:E:145:VAL:HG21	1.84	0.58
1:D:58:ILE:CD1	1:D:84:LEU:HD11	2.33	0.58
1:B:15:ALA:HB2	1:B:145:VAL:HG21	1.85	0.58
1:E:77:LEU:C	1:E:79:LYS:H	2.11	0.58
1:C:98:ARG:O	1:C:98:ARG:HD3	2.03	0.58
1:B:242:CYS:O	1:B:244:PRO:HD3	2.03	0.58
1:C:207:PHE:CE2	1:C:390:GLY:HA3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:CD1	1:A:84:LEU:HD11	2.34	0.58
1:B:98:ARG:HD3	1:B:98:ARG:O	2.04	0.58
1:D:14:LEU:HD21	1:D:246:LEU:CD1	2.28	0.58
1:B:207:PHE:CE2	1:B:390:GLY:HA3	2.38	0.58
1:B:217:THR:HG23	1:B:264:VAL:HA	1.86	0.58
1:E:40:VAL:HG21	1:E:59:TYR:CE1	2.39	0.58
1:A:40:VAL:HG21	1:A:59:TYR:CE1	2.36	0.57
1:B:260:VAL:O	1:B:284:PHE:HB3	2.04	0.57
1:D:236:THR:HB	1:D:240:ARG:HB3	1.85	0.57
1:E:242:CYS:O	1:E:244:PRO:HD3	2.04	0.57
1:C:77:LEU:C	1:C:79:LYS:H	2.12	0.57
1:C:206:ARG:HH11	1:C:227:HIS:CE1	2.22	0.57
1:C:293:ARG:HB3	1:C:293:ARG:HH11	1.68	0.57
1:C:77:LEU:H	1:C:77:LEU:HD12	1.68	0.57
1:E:217:THR:HG23	1:E:264:VAL:HA	1.86	0.57
1:A:236:THR:HB	1:A:240:ARG:HB3	1.86	0.57
1:B:159:GLY:O	1:B:160:LEU:C	2.47	0.57
1:C:285:GLU:O	1:C:286:ARG:HG2	2.04	0.57
1:E:153:ALA:HB1	1:E:165:ALA:CB	2.34	0.57
1:D:34:ILE:HD12	1:E:59:TYR:HE2	1.70	0.57
1:C:160:LEU:HB2	1:C:161:PRO:HD3	1.87	0.57
1:C:236:THR:HB	1:C:240:ARG:HB3	1.86	0.57
1:A:77:LEU:HD12	1:A:77:LEU:H	1.70	0.57
1:B:153:ALA:HB1	1:B:165:ALA:CB	2.34	0.57
1:A:84:LEU:O	1:A:88:MET:HG3	2.04	0.57
1:A:48:TYR:HA	1:A:52:ALA:HB3	1.87	0.56
1:A:380:MET:SD	1:A:380:MET:N	2.78	0.56
1:D:380:MET:SD	1:D:380:MET:N	2.78	0.56
1:E:293:ARG:HB3	1:E:293:ARG:HH11	1.69	0.56
1:A:293:ARG:HB3	1:A:293:ARG:HH11	1.69	0.56
1:D:84:LEU:O	1:D:88:MET:HG3	2.05	0.56
1:D:144:ILE:CG2	1:D:337:LEU:HD22	2.35	0.56
1:D:217:THR:HG23	1:D:264:VAL:HA	1.88	0.56
1:C:40:VAL:HG21	1:C:59:TYR:CE1	2.39	0.56
1:D:184:PRO:C	1:D:185:ILE:HG13	2.30	0.56
1:D:234:THR:HG22	1:D:235:ALA:N	2.21	0.56
1:E:84:LEU:O	1:E:88:MET:HG3	2.06	0.56
1:A:348:PHE:CE1	1:A:379:TRP:NE1	2.74	0.56
1:E:48:TYR:HA	1:E:52:ALA:HB3	1.88	0.56
1:B:206:ARG:HH11	1:B:227:HIS:CE1	2.24	0.56
1:B:285:GLU:O	1:B:286:ARG:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD12	1:D:77:LEU:H	1.71	0.56
1:A:98:ARG:O	1:A:98:ARG:HD3	2.05	0.56
1:A:293:ARG:HE	1:E:206:ARG:HH21	1.52	0.56
1:B:170:TRP:CD1	1:B:171:GLU:N	2.73	0.56
1:A:234:THR:HG22	1:A:235:ALA:N	2.21	0.55
1:B:40:VAL:HG21	1:B:59:TYR:CE1	2.39	0.55
1:B:160:LEU:HB2	1:B:161:PRO:HD3	1.88	0.55
1:E:206:ARG:HH11	1:E:227:HIS:CE1	2.24	0.55
1:B:77:LEU:HD12	1:B:77:LEU:H	1.70	0.55
1:C:15:ALA:HB2	1:C:145:VAL:HG21	1.87	0.55
1:D:77:LEU:C	1:D:79:LYS:H	2.15	0.55
1:E:260:VAL:O	1:E:284:PHE:HB3	2.05	0.55
1:A:77:LEU:C	1:A:79:LYS:H	2.13	0.55
1:D:293:ARG:HB3	1:D:293:ARG:HH11	1.71	0.55
1:E:160:LEU:HB2	1:E:161:PRO:HD3	1.88	0.55
1:A:159:GLY:O	1:A:160:LEU:C	2.49	0.55
1:A:217:THR:HG23	1:A:264:VAL:HA	1.88	0.55
1:B:18:VAL:CG2	1:B:185:ILE:HG23	2.36	0.55
1:C:77:LEU:HD12	1:C:77:LEU:N	2.22	0.55
1:D:160:LEU:HB2	1:D:161:PRO:HD3	1.87	0.55
1:D:245:ASN:HB2	1:D:248:THR:OG1	2.07	0.55
1:D:15:ALA:HB2	1:D:145:VAL:HG21	1.87	0.55
1:D:159:GLY:O	1:D:160:LEU:C	2.50	0.55
1:A:185:ILE:H	1:A:185:ILE:CD1	2.13	0.55
1:B:8:LEU:HD13	1:B:8:LEU:O	2.07	0.55
1:B:77:LEU:C	1:B:79:LYS:H	2.15	0.55
1:D:48:TYR:HA	1:D:52:ALA:HB3	1.88	0.55
1:B:153:ALA:HB1	1:B:165:ALA:C	2.32	0.55
1:C:380:MET:SD	1:C:380:MET:N	2.80	0.55
1:B:167:ARG:HA	1:B:170:TRP:CE2	2.42	0.54
1:C:84:LEU:O	1:C:88:MET:HG3	2.07	0.54
1:E:77:LEU:HD12	1:E:77:LEU:H	1.73	0.54
1:A:265:ARG:HD2	1:E:392:TYR:HE2	1.72	0.54
1:B:176:ALA:HB3	1:B:338:PHE:CZ	2.42	0.54
1:D:206:ARG:HH11	1:D:227:HIS:CE1	2.25	0.54
1:E:98:ARG:O	1:E:98:ARG:HD3	2.07	0.54
1:D:285:GLU:O	1:D:286:ARG:HG2	2.08	0.54
1:D:348:PHE:CE1	1:D:379:TRP:NE1	2.76	0.54
1:D:143:THR:HA	1:D:244:PRO:O	2.07	0.54
1:E:147:PHE:CZ	1:E:170:TRP:CB	2.89	0.54
1:E:159:GLY:O	1:E:160:LEU:C	2.49	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:THR:CG2	1:A:246:LEU:HD23	2.38	0.54
1:C:339:ASP:HB3	1:C:380:MET:CE	2.37	0.54
1:B:48:TYR:HA	1:B:52:ALA:HB3	1.89	0.54
1:C:348:PHE:CE1	1:C:379:TRP:NE1	2.76	0.54
1:A:15:ALA:HB2	1:A:145:VAL:HG21	1.88	0.54
1:C:206:ARG:NH2	1:D:293:ARG:HE	1.85	0.54
1:C:392:TYR:HE2	1:D:265:ARG:HD2	1.71	0.54
1:E:40:VAL:HG11	1:E:57:VAL:HG11	1.90	0.54
1:E:167:ARG:HA	1:E:170:TRP:CE2	2.43	0.54
1:B:140:THR:O	1:B:236:THR:CG2	2.50	0.53
1:C:153:ALA:HB1	1:C:165:ALA:C	2.33	0.53
1:C:167:ARG:HA	1:C:170:TRP:CE2	2.43	0.53
1:E:241:LEU:HD12	1:E:241:LEU:N	2.22	0.53
1:D:37:VAL:HG13	1:E:34:ILE:HD11	1.90	0.53
1:E:170:TRP:CD1	1:E:171:GLU:N	2.76	0.53
1:E:380:MET:SD	1:E:380:MET:N	2.81	0.53
1:D:98:ARG:O	1:D:98:ARG:HD3	2.06	0.53
1:A:206:ARG:HH11	1:A:227:HIS:CE1	2.26	0.53
1:D:16:ILE:HD12	1:D:16:ILE:N	2.23	0.53
1:D:170:TRP:CD1	1:D:171:GLU:N	2.75	0.53
1:E:348:PHE:CE1	1:E:379:TRP:NE1	2.77	0.53
1:B:348:PHE:CE1	1:B:379:TRP:NE1	2.77	0.53
1:C:30:ALA:HB3	1:C:57:VAL:HG12	1.91	0.53
1:A:285:GLU:O	1:A:286:ARG:CG	2.57	0.53
1:A:77:LEU:HD12	1:A:77:LEU:N	2.24	0.53
1:C:170:TRP:CD1	1:C:171:GLU:N	2.75	0.53
1:D:153:ALA:HB1	1:D:165:ALA:C	2.33	0.53
1:A:14:LEU:HD21	1:A:246:LEU:HD11	1.91	0.53
1:C:147:PHE:CD2	1:C:148:ALA:N	2.77	0.53
1:D:37:VAL:CG1	1:E:34:ILE:HD11	2.39	0.53
1:C:143:THR:CG2	1:C:246:LEU:HD23	2.38	0.52
1:D:40:VAL:HG11	1:D:57:VAL:HG11	1.92	0.52
1:D:146:PRO:HG3	1:D:338:PHE:HE1	1.72	0.52
1:E:153:ALA:HB1	1:E:165:ALA:C	2.35	0.52
1:A:153:ALA:HB1	1:A:165:ALA:C	2.34	0.52
1:A:170:TRP:CD1	1:A:171:GLU:N	2.76	0.52
1:E:245:ASN:ND2	1:E:337:LEU:HD13	2.25	0.52
1:E:284:PHE:CE1	1:E:289:ALA:HB2	2.44	0.52
1:E:339:ASP:HB3	1:E:380:MET:CE	2.39	0.52
1:C:159:GLY:O	1:C:160:LEU:C	2.52	0.52
1:D:339:ASP:HB3	1:D:380:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:LEU:HD12	1:E:26:GLN:OE1	2.09	0.52
1:A:40:VAL:HG11	1:A:57:VAL:HG11	1.91	0.52
1:B:40:VAL:HG11	1:B:57:VAL:HG11	1.90	0.52
1:B:84:LEU:O	1:B:88:MET:HG3	2.08	0.52
1:B:234:THR:HG22	1:B:235:ALA:N	2.25	0.52
1:C:8:LEU:HD13	1:C:8:LEU:O	2.10	0.52
1:C:200:ALA:HB1	1:D:295:GLU:O	2.09	0.52
1:E:245:ASN:HB2	1:E:248:THR:OG1	2.10	0.52
1:A:265:ARG:NH1	1:E:392:TYR:CE2	2.78	0.52
1:A:265:ARG:CZ	1:E:392:TYR:HD2	2.23	0.52
1:A:167:ARG:HA	1:A:170:TRP:CE2	2.45	0.52
1:A:339:ASP:HB3	1:A:380:MET:CE	2.39	0.52
1:C:22:LEU:HD12	1:C:26:GLN:OE1	2.09	0.52
1:C:61:ASP:OD1	1:C:63:GLU:N	2.42	0.52
1:D:317:VAL:HA	1:D:346:ILE:HD12	1.92	0.52
1:A:61:ASP:OD1	1:A:63:GLU:N	2.43	0.52
1:A:241:LEU:HD12	1:A:241:LEU:N	2.24	0.52
1:B:339:ASP:HB3	1:B:380:MET:CE	2.40	0.52
1:C:245:ASN:HB2	1:C:248:THR:OG1	2.09	0.52
1:A:81:PRO:HG3	1:B:54:LEU:HD21	1.92	0.52
1:A:245:ASN:HB2	1:A:248:THR:OG1	2.09	0.52
1:E:281:PHE:CD1	1:E:282:ALA:N	2.78	0.52
1:D:77:LEU:HD12	1:D:77:LEU:N	2.25	0.51
1:E:234:THR:HG22	1:E:235:ALA:N	2.25	0.51
1:A:30:ALA:HB3	1:A:57:VAL:HG12	1.93	0.51
1:C:217:THR:HG23	1:C:264:VAL:HA	1.91	0.51
1:D:61:ASP:OD1	1:D:63:GLU:N	2.43	0.51
1:B:147:PHE:CZ	1:B:170:TRP:CB	2.90	0.51
1:C:234:THR:HG22	1:C:235:ALA:N	2.24	0.51
1:B:139:VAL:C	1:B:236:THR:CG2	2.83	0.51
1:C:206:ARG:NH2	1:D:293:ARG:CD	2.69	0.51
1:E:16:ILE:N	1:E:16:ILE:HD12	2.26	0.51
1:B:61:ASP:OD1	1:B:63:GLU:N	2.43	0.51
1:B:147:PHE:CD2	1:B:148:ALA:N	2.79	0.51
1:C:40:VAL:HG11	1:C:57:VAL:HG11	1.91	0.51
1:C:147:PHE:CZ	1:C:170:TRP:CB	2.90	0.51
1:D:167:ARG:HA	1:D:170:TRP:CE2	2.46	0.51
1:B:22:LEU:HD12	1:B:26:GLN:OE1	2.10	0.51
1:B:137:GLU:O	1:B:139:VAL:HG13	2.11	0.51
1:C:48:TYR:HA	1:C:52:ALA:HB3	1.92	0.51
1:D:22:LEU:HD12	1:D:26:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:C	1:B:197:GLU:N	2.69	0.51
1:B:380:MET:SD	1:B:380:MET:N	2.84	0.51
1:A:43:LEU:O	1:A:44:ALA:C	2.54	0.51
1:C:245:ASN:ND2	1:C:337:LEU:HD13	2.26	0.51
1:B:43:LEU:O	1:B:44:ALA:C	2.53	0.51
1:B:317:VAL:HA	1:B:346:ILE:HD12	1.93	0.51
1:C:247:PRO:HB3	1:C:326:ILE:HD11	1.92	0.51
1:B:77:LEU:HD12	1:B:77:LEU:N	2.25	0.50
1:B:373:SER:OG	1:B:374:LEU:N	2.44	0.50
1:C:392:TYR:HD2	1:D:265:ARG:CZ	2.24	0.50
1:E:247:PRO:HB3	1:E:326:ILE:HD11	1.94	0.50
1:E:265:ARG:HG3	1:E:281:PHE:HB2	1.93	0.50
1:A:147:PHE:CD2	1:A:148:ALA:N	2.79	0.50
1:B:281:PHE:CD1	1:B:282:ALA:N	2.79	0.50
1:A:22:LEU:HD12	1:A:26:GLN:OE1	2.11	0.50
1:A:247:PRO:HB3	1:A:326:ILE:HD11	1.92	0.50
1:B:284:PHE:CE1	1:B:289:ALA:HB2	2.46	0.50
1:C:43:LEU:O	1:C:44:ALA:C	2.54	0.50
1:D:14:LEU:C	1:D:14:LEU:CD2	2.80	0.50
1:A:51:GLY:O	1:A:52:ALA:C	2.55	0.50
1:A:245:ASN:ND2	1:A:337:LEU:HD13	2.27	0.50
1:C:16:ILE:N	1:C:16:ILE:HD12	2.26	0.50
1:E:51:GLY:O	1:E:52:ALA:C	2.54	0.50
1:A:266:ALA:CB	1:A:280:ILE:HG23	2.42	0.50
1:D:101:VAL:HA	1:D:145:VAL:O	2.11	0.50
1:E:143:THR:CG2	1:E:246:LEU:HD21	2.42	0.50
1:B:241:LEU:HD12	1:B:241:LEU:N	2.24	0.50
1:C:101:VAL:HA	1:C:145:VAL:O	2.12	0.50
1:C:285:GLU:O	1:C:286:ARG:CG	2.60	0.50
1:E:61:ASP:OD1	1:E:63:GLU:N	2.45	0.50
1:E:147:PHE:CD2	1:E:148:ALA:N	2.80	0.50
1:E:195:LEU:C	1:E:197:GLU:N	2.69	0.50
1:D:290:VAL:HG12	1:D:290:VAL:O	2.11	0.50
1:A:14:LEU:C	1:A:14:LEU:CD2	2.85	0.50
1:A:147:PHE:CZ	1:A:170:TRP:CB	2.91	0.50
1:A:160:LEU:CB	1:A:161:PRO:HD3	2.42	0.50
1:A:195:LEU:C	1:A:197:GLU:N	2.69	0.50
1:B:164:GLU:CA	1:B:167:ARG:HB2	2.33	0.50
1:B:265:ARG:HG3	1:B:281:PHE:HB2	1.94	0.50
1:D:284:PHE:CE1	1:D:289:ALA:HB2	2.47	0.50
1:E:30:ALA:HB3	1:E:57:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HA	1:A:145:VAL:O	2.12	0.49
1:B:51:GLY:O	1:B:52:ALA:C	2.54	0.49
1:B:171:GLU:HA	1:B:174:PHE:HD2	1.77	0.49
1:C:51:GLY:O	1:C:52:ALA:C	2.55	0.49
1:D:147:PHE:CD2	1:D:148:ALA:N	2.80	0.49
1:D:153:ALA:HB1	1:D:165:ALA:HB1	1.94	0.49
1:E:245:ASN:HD22	1:E:337:LEU:HD13	1.77	0.49
1:C:153:ALA:O	1:C:165:ALA:HB1	2.12	0.49
1:C:392:TYR:CD2	1:D:265:ARG:CZ	2.96	0.49
1:B:290:VAL:HG12	1:B:290:VAL:O	2.13	0.49
1:C:153:ALA:HB1	1:C:165:ALA:HB1	1.94	0.49
1:D:30:ALA:HB3	1:D:57:VAL:HG12	1.94	0.49
1:B:245:ASN:HB2	1:B:248:THR:OG1	2.13	0.49
1:C:39:PHE:O	1:C:40:VAL:C	2.55	0.49
1:C:195:LEU:O	1:C:199:VAL:HG23	2.13	0.49
1:B:266:ALA:CB	1:B:280:ILE:HG23	2.40	0.49
1:D:195:LEU:O	1:D:199:VAL:HG23	2.12	0.49
1:E:8:LEU:HD13	1:E:8:LEU:O	2.12	0.49
1:B:16:ILE:N	1:B:16:ILE:HD12	2.28	0.49
1:B:245:ASN:ND2	1:B:337:LEU:HD13	2.27	0.49
1:C:143:THR:HG21	1:C:246:LEU:CD2	2.43	0.49
1:D:281:PHE:CD1	1:D:282:ALA:N	2.81	0.49
1:E:77:LEU:HD12	1:E:77:LEU:N	2.26	0.49
1:E:285:GLU:O	1:E:286:ARG:CG	2.60	0.49
1:E:317:VAL:HA	1:E:346:ILE:HD12	1.93	0.49
1:B:247:PRO:HB3	1:B:326:ILE:HD11	1.94	0.49
1:C:245:ASN:HD22	1:C:337:LEU:HD13	1.78	0.49
1:E:43:LEU:O	1:E:44:ALA:C	2.56	0.49
1:B:30:ALA:HB3	1:B:57:VAL:HG12	1.95	0.49
1:A:265:ARG:HG3	1:A:281:PHE:HB2	1.93	0.49
1:A:281:PHE:CD1	1:A:282:ALA:N	2.81	0.49
1:E:77:LEU:O	1:E:79:LYS:N	2.46	0.49
1:D:43:LEU:O	1:D:44:ALA:C	2.56	0.49
1:D:51:GLY:O	1:D:52:ALA:C	2.56	0.49
1:D:241:LEU:HD12	1:D:241:LEU:N	2.26	0.48
1:B:17:ARG:HB3	1:B:185:ILE:HG23	1.87	0.48
1:D:247:PRO:HB3	1:D:326:ILE:HD11	1.95	0.48
1:E:14:LEU:C	1:E:14:LEU:CD2	2.84	0.48
1:E:185:ILE:HD12	1:E:185:ILE:N	2.28	0.48
1:A:16:ILE:HD12	1:A:16:ILE:N	2.26	0.48
1:B:101:VAL:HA	1:B:145:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PHE:CD1	1:C:282:ALA:N	2.81	0.48
1:B:188:TRP:CH2	1:B:246:LEU:O	2.67	0.48
1:B:245:ASN:HD22	1:B:337:LEU:HD13	1.78	0.48
1:D:245:ASN:ND2	1:D:337:LEU:HD13	2.28	0.48
1:E:171:GLU:HA	1:E:174:PHE:HD2	1.77	0.48
1:E:290:VAL:HG12	1:E:290:VAL:O	2.12	0.48
1:C:171:GLU:HA	1:C:174:PHE:HD2	1.77	0.48
1:D:184:PRO:HG2	1:D:185:ILE:HD11	1.96	0.48
1:D:184:PRO:O	1:D:185:ILE:HG13	2.12	0.48
1:E:101:VAL:HA	1:E:145:VAL:O	2.13	0.48
1:A:77:LEU:O	1:A:79:LYS:N	2.46	0.48
1:D:39:PHE:O	1:D:40:VAL:C	2.55	0.48
1:E:164:GLU:CA	1:E:167:ARG:HB2	2.35	0.48
1:A:290:VAL:HG12	1:A:290:VAL:O	2.13	0.48
1:A:373:SER:OG	1:A:374:LEU:N	2.47	0.48
1:C:77:LEU:O	1:C:79:LYS:N	2.46	0.48
1:C:164:GLU:CA	1:C:167:ARG:HB2	2.34	0.48
1:C:266:ALA:CB	1:C:280:ILE:HG23	2.43	0.48
1:D:171:GLU:HA	1:D:174:PHE:HD2	1.79	0.48
1:E:153:ALA:HB1	1:E:165:ALA:HB1	1.96	0.48
1:A:317:VAL:HA	1:A:346:ILE:HD12	1.95	0.48
1:D:147:PHE:CZ	1:D:170:TRP:CB	2.92	0.48
1:D:219:LEU:HD11	1:D:260:VAL:HG12	1.96	0.48
1:E:39:PHE:O	1:E:40:VAL:C	2.56	0.48
1:E:58:ILE:HD13	1:E:84:LEU:HD11	1.95	0.48
1:E:160:LEU:CB	1:E:161:PRO:HD3	2.44	0.48
1:A:153:ALA:HB1	1:A:165:ALA:HB1	1.94	0.48
1:A:265:ARG:CZ	1:E:392:TYR:CD2	2.97	0.48
1:C:265:ARG:HG3	1:C:281:PHE:HB2	1.95	0.48
1:D:265:ARG:HG3	1:D:281:PHE:HB2	1.96	0.48
1:C:195:LEU:C	1:C:197:GLU:N	2.70	0.47
1:A:39:PHE:O	1:A:40:VAL:C	2.57	0.47
1:B:280:ILE:HG12	1:B:379:TRP:CZ3	2.49	0.47
1:D:195:LEU:C	1:D:197:GLU:N	2.71	0.47
1:A:37:VAL:HG13	1:B:34:ILE:HD11	1.96	0.47
1:B:14:LEU:C	1:B:14:LEU:CD2	2.82	0.47
1:C:392:TYR:CE2	1:D:265:ARG:NH1	2.82	0.47
1:E:152:TRP:CZ3	1:E:169:LEU:HD11	2.49	0.47
1:A:348:PHE:HE1	1:A:379:TRP:NE1	2.12	0.47
1:C:143:THR:HG21	1:C:246:LEU:HD21	1.94	0.47
1:C:284:PHE:CE1	1:C:289:ALA:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:PHE:O	1:B:40:VAL:C	2.56	0.47
1:E:346:ILE:HD12	1:E:346:ILE:HA	1.74	0.47
1:A:245:ASN:HD22	1:A:337:LEU:HD13	1.80	0.47
1:B:17:ARG:CB	1:B:185:ILE:HG21	2.29	0.47
1:D:264:VAL:HG13	1:D:264:VAL:O	2.15	0.47
1:D:373:SER:OG	1:D:374:LEU:N	2.48	0.47
1:E:44:ALA:O	1:E:45:GLU:C	2.58	0.47
1:A:8:LEU:O	1:A:8:LEU:HD13	2.14	0.47
1:A:55:PHE:CE2	1:A:57:VAL:CG1	2.98	0.47
1:A:210:LEU:HD12	1:A:317:VAL:HG11	1.97	0.47
1:B:44:ALA:O	1:B:45:GLU:C	2.58	0.47
1:B:293:ARG:HH11	1:B:293:ARG:CB	2.28	0.47
1:C:264:VAL:HG13	1:C:264:VAL:O	2.14	0.47
1:C:336:THR:O	1:C:337:LEU:C	2.55	0.47
1:D:137:GLU:O	1:D:139:VAL:HG13	2.14	0.47
1:D:153:ALA:O	1:D:165:ALA:HB1	2.15	0.47
1:E:144:ILE:O	1:E:246:LEU:HD23	2.14	0.47
1:E:336:THR:O	1:E:337:LEU:C	2.58	0.47
1:A:164:GLU:CA	1:A:167:ARG:HB2	2.34	0.47
1:B:160:LEU:O	1:B:161:PRO:C	2.57	0.47
1:C:317:VAL:HA	1:C:346:ILE:HD12	1.95	0.47
1:C:373:SER:OG	1:C:374:LEU:N	2.48	0.47
1:D:19:GLY:C	1:D:143:THR:OG1	2.58	0.47
1:D:184:PRO:CD	1:D:185:ILE:CD1	2.86	0.47
1:C:137:GLU:O	1:C:139:VAL:HG13	2.15	0.47
1:D:160:LEU:CB	1:D:161:PRO:HD3	2.45	0.47
1:E:188:TRP:CH2	1:E:246:LEU:O	2.68	0.47
1:C:160:LEU:CB	1:C:161:PRO:HD3	2.45	0.47
1:C:241:LEU:HD12	1:C:241:LEU:N	2.27	0.47
1:A:137:GLU:O	1:A:139:VAL:HG13	2.15	0.46
1:A:284:PHE:CE1	1:A:289:ALA:HB2	2.50	0.46
1:B:58:ILE:HD13	1:B:84:LEU:HD11	1.96	0.46
1:D:8:LEU:HD13	1:D:8:LEU:O	2.15	0.46
1:C:33:PRO:O	1:C:35:GLU:N	2.48	0.46
1:C:290:VAL:HG12	1:C:290:VAL:O	2.16	0.46
1:D:356:LEU:HD12	1:D:365:PHE:CE1	2.50	0.46
1:E:185:ILE:H	1:E:185:ILE:CD1	2.22	0.46
1:E:281:PHE:CD1	1:E:281:PHE:C	2.93	0.46
1:A:37:VAL:CG1	1:B:34:ILE:HD11	2.45	0.46
1:B:149:HIS:C	1:B:151:GLY:N	2.73	0.46
1:C:204:ALA:HB2	1:D:294:ALA:C	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:GLU:O	1:E:139:VAL:HG13	2.15	0.46
1:E:285:GLU:C	1:E:286:ARG:HG2	2.40	0.46
1:B:153:ALA:HB1	1:B:165:ALA:HB1	1.97	0.46
1:C:293:ARG:HH11	1:C:293:ARG:CB	2.28	0.46
1:A:336:THR:O	1:A:337:LEU:C	2.58	0.46
1:E:266:ALA:CB	1:E:280:ILE:HG23	2.43	0.46
1:A:19:GLY:C	1:A:143:THR:OG1	2.59	0.46
1:A:152:TRP:CZ3	1:A:169:LEU:HD11	2.49	0.46
1:D:146:PRO:HG3	1:D:338:PHE:CE1	2.50	0.46
1:D:285:GLU:O	1:D:286:ARG:CG	2.64	0.46
1:E:22:LEU:HD11	1:E:26:GLN:HB3	1.97	0.46
1:A:251:VAL:HG23	1:A:251:VAL:O	2.15	0.46
1:B:143:THR:CG2	1:B:144:ILE:N	2.61	0.46
1:C:281:PHE:CD1	1:C:281:PHE:C	2.94	0.46
1:D:333:PHE:O	1:D:334:PHE:C	2.58	0.46
1:A:89:ALA:O	1:A:90:ARG:C	2.59	0.46
1:B:160:LEU:CB	1:B:161:PRO:HD3	2.45	0.46
1:C:19:GLY:C	1:C:143:THR:OG1	2.59	0.46
1:D:106:PRO:HD3	1:D:334:PHE:HB2	1.97	0.46
1:D:143:THR:HG23	1:D:244:PRO:O	2.16	0.46
1:E:160:LEU:O	1:E:161:PRO:C	2.59	0.46
1:E:264:VAL:HG13	1:E:264:VAL:O	2.16	0.46
1:A:195:LEU:O	1:A:199:VAL:HG23	2.16	0.46
1:B:152:TRP:CZ3	1:B:169:LEU:HD11	2.51	0.46
1:B:195:LEU:O	1:B:199:VAL:HG23	2.16	0.46
1:B:195:LEU:O	1:B:197:GLU:N	2.49	0.46
1:D:160:LEU:O	1:D:161:PRO:C	2.59	0.46
1:E:373:SER:OG	1:E:374:LEU:N	2.46	0.46
1:C:89:ALA:O	1:C:90:ARG:C	2.59	0.46
1:D:220:VAL:O	1:D:220:VAL:HG12	2.15	0.46
1:A:195:LEU:O	1:A:197:GLU:N	2.49	0.45
1:B:210:LEU:HD12	1:B:317:VAL:HG11	1.97	0.45
1:C:44:ALA:O	1:C:45:GLU:C	2.59	0.45
1:D:188:TRP:CH2	1:D:246:LEU:O	2.69	0.45
1:D:155:ALA:HB1	1:D:334:PHE:CE2	2.51	0.45
1:D:164:GLU:CA	1:D:167:ARG:HB2	2.33	0.45
1:D:281:PHE:CD1	1:D:281:PHE:C	2.93	0.45
1:E:19:GLY:C	1:E:143:THR:OG1	2.59	0.45
1:A:264:VAL:HG13	1:A:264:VAL:O	2.15	0.45
1:B:285:GLU:O	1:B:286:ARG:CG	2.63	0.45
1:C:22:LEU:HD11	1:C:26:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:LEU:HD12	1:C:365:PHE:CE1	2.51	0.45
1:D:58:ILE:HD13	1:D:84:LEU:HD11	1.98	0.45
1:D:251:VAL:HG23	1:D:251:VAL:O	2.15	0.45
1:B:33:PRO:C	1:B:35:GLU:H	2.24	0.45
1:C:241:LEU:O	1:C:242:CYS:HB3	2.16	0.45
1:D:77:LEU:O	1:D:79:LYS:N	2.49	0.45
1:D:336:THR:O	1:D:337:LEU:C	2.59	0.45
1:E:195:LEU:O	1:E:197:GLU:N	2.49	0.45
1:E:356:LEU:HD12	1:E:365:PHE:CE1	2.52	0.45
1:A:160:LEU:O	1:A:161:PRO:C	2.60	0.45
1:B:208:HIS:O	1:B:209:ALA:HB2	2.16	0.45
1:C:58:ILE:HD13	1:C:84:LEU:HD11	1.97	0.45
1:C:210:LEU:HD12	1:C:317:VAL:HG11	1.99	0.45
1:D:74:GLU:C	1:D:76:GLY:N	2.75	0.45
1:A:10:LYS:O	1:A:11:LEU:C	2.58	0.45
1:B:33:PRO:O	1:B:35:GLU:N	2.50	0.45
1:C:14:LEU:C	1:C:14:LEU:CD2	2.82	0.45
1:C:188:TRP:CH2	1:C:246:LEU:O	2.70	0.45
1:C:285:GLU:C	1:C:286:ARG:HG2	2.41	0.45
1:D:89:ALA:O	1:D:90:ARG:C	2.59	0.45
1:E:33:PRO:O	1:E:35:GLU:N	2.50	0.45
1:E:149:HIS:O	1:E:151:GLY:N	2.50	0.45
1:A:265:ARG:NH1	1:E:392:TYR:HD2	2.13	0.45
1:A:281:PHE:CD1	1:A:281:PHE:C	2.95	0.45
1:A:293:ARG:HH11	1:A:293:ARG:CB	2.29	0.45
1:B:241:LEU:O	1:B:242:CYS:HB3	2.15	0.45
1:D:22:LEU:HD11	1:D:26:GLN:HB3	1.98	0.45
1:D:34:ILE:HD11	1:E:37:VAL:HG13	1.99	0.45
1:A:171:GLU:HA	1:A:174:PHE:HD2	1.80	0.45
1:B:336:THR:O	1:B:337:LEU:C	2.58	0.45
1:A:92:PHE:CE2	1:A:98:ARG:HB2	2.51	0.45
1:B:22:LEU:HD11	1:B:26:GLN:HB3	1.98	0.45
1:B:35:GLU:H	1:B:35:GLU:HG2	1.48	0.45
1:B:251:VAL:O	1:B:251:VAL:HG23	2.16	0.45
1:C:152:TRP:CZ3	1:C:169:LEU:HD11	2.51	0.45
1:D:152:TRP:CZ3	1:D:169:LEU:HD11	2.52	0.45
1:A:88:MET:HE2	1:A:88:MET:HB3	1.90	0.44
1:A:188:TRP:CH2	1:A:246:LEU:O	2.70	0.44
1:B:77:LEU:O	1:B:79:LYS:N	2.50	0.44
1:B:346:ILE:HD12	1:B:346:ILE:HA	1.72	0.44
1:C:208:HIS:O	1:C:209:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PRO:C	1:A:35:GLU:H	2.25	0.44
1:B:19:GLY:C	1:B:143:THR:OG1	2.60	0.44
1:C:33:PRO:C	1:C:35:GLU:H	2.25	0.44
1:E:33:PRO:C	1:E:35:GLU:H	2.25	0.44
1:E:143:THR:CG2	1:E:246:LEU:CD2	2.96	0.44
1:E:280:ILE:HG12	1:E:379:TRP:CZ3	2.52	0.44
1:C:148:ALA:O	1:C:149:HIS:HB2	2.18	0.44
1:E:32:ALA:HA	1:E:33:PRO:HD3	1.82	0.44
1:E:77:LEU:C	1:E:79:LYS:N	2.75	0.44
1:A:272:LEU:HD11	1:A:304:LEU:HD22	2.00	0.44
1:A:346:ILE:HD12	1:A:346:ILE:HA	1.73	0.44
1:A:113:PRO:HA	1:A:114:PRO:HD3	1.82	0.44
1:A:153:ALA:O	1:A:165:ALA:HB1	2.18	0.44
1:A:285:GLU:C	1:A:286:ARG:HG2	2.41	0.44
1:C:20:LEU:HD23	1:C:143:THR:OG1	2.18	0.44
1:C:77:LEU:H	1:C:77:LEU:CD1	2.31	0.44
1:C:280:ILE:HG12	1:C:379:TRP:CZ3	2.52	0.44
1:E:145:VAL:HG12	1:E:146:PRO:N	2.32	0.44
1:E:195:LEU:O	1:E:199:VAL:HG23	2.18	0.44
1:C:160:LEU:O	1:C:161:PRO:C	2.60	0.44
1:C:280:ILE:HG13	1:C:281:PHE:N	2.32	0.44
1:E:20:LEU:HD23	1:E:143:THR:OG1	2.18	0.44
1:B:32:ALA:HA	1:B:33:PRO:HD3	1.81	0.44
1:B:153:ALA:O	1:B:165:ALA:HB1	2.18	0.44
1:D:356:LEU:HD23	1:D:356:LEU:HA	1.75	0.44
1:B:131:ALA:O	1:B:132:LEU:C	2.61	0.44
1:B:140:THR:N	1:B:236:THR:CG2	2.80	0.44
1:B:356:LEU:HD12	1:B:365:PHE:CE1	2.53	0.44
1:C:206:ARG:HG2	1:D:281:PHE:CE2	2.53	0.44
1:D:348:PHE:HE1	1:D:379:TRP:NE1	2.15	0.44
1:E:161:PRO:O	1:E:165:ALA:N	2.51	0.44
1:A:265:ARG:CD	1:E:392:TYR:HE2	2.31	0.44
1:A:388:VAL:HB	1:A:401:MET:HB2	2.00	0.44
1:B:149:HIS:O	1:B:151:GLY:N	2.51	0.44
1:C:74:GLU:C	1:C:76:GLY:N	2.76	0.44
1:D:44:ALA:O	1:D:45:GLU:C	2.59	0.44
1:E:149:HIS:C	1:E:151:GLY:N	2.72	0.44
1:E:220:VAL:O	1:E:220:VAL:HG12	2.17	0.44
1:A:20:LEU:HD23	1:A:143:THR:OG1	2.17	0.43
1:A:148:ALA:O	1:A:149:HIS:HB2	2.17	0.43
1:D:185:ILE:HD12	1:D:185:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:O	1:E:11:LEU:C	2.61	0.43
1:C:195:LEU:O	1:C:197:GLU:N	2.51	0.43
1:D:202:LEU:HD13	1:D:229:TRP:CZ3	2.54	0.43
1:D:245:ASN:HD22	1:D:337:LEU:HD13	1.83	0.43
1:D:285:GLU:C	1:D:286:ARG:HG2	2.43	0.43
1:D:332:VAL:O	1:D:334:PHE:CE2	2.71	0.43
1:D:389:ASP:OD1	1:D:402:ARG:NH2	2.48	0.43
1:E:210:LEU:HD12	1:E:317:VAL:HG11	2.00	0.43
1:E:293:ARG:HH11	1:E:293:ARG:CB	2.31	0.43
1:B:139:VAL:N	1:B:236:THR:HG23	2.33	0.43
1:B:281:PHE:CD1	1:B:281:PHE:C	2.92	0.43
1:B:285:GLU:C	1:B:286:ARG:HG2	2.43	0.43
1:D:208:HIS:O	1:D:209:ALA:HB2	2.18	0.43
1:E:131:ALA:O	1:E:132:LEU:C	2.61	0.43
1:A:74:GLU:C	1:A:76:GLY:N	2.76	0.43
1:A:343:ALA:O	1:A:344:SER:C	2.60	0.43
1:B:272:LEU:HD11	1:B:304:LEU:HD22	2.00	0.43
1:A:33:PRO:O	1:A:35:GLU:N	2.52	0.43
1:B:161:PRO:O	1:B:165:ALA:N	2.51	0.43
1:C:348:PHE:HE1	1:C:379:TRP:NE1	2.16	0.43
1:D:157:PHE:C	1:D:159:GLY:H	2.26	0.43
1:D:330:GLY:O	1:D:331:LEU:HD23	2.18	0.43
1:A:44:ALA:O	1:A:45:GLU:C	2.61	0.43
1:A:352:TYR:HB3	1:A:354:GLU:CG	2.47	0.43
1:B:332:VAL:O	1:B:334:PHE:CE2	2.71	0.43
1:C:330:GLY:O	1:C:331:LEU:HD23	2.18	0.43
1:D:33:PRO:C	1:D:35:GLU:H	2.26	0.43
1:D:333:PHE:O	1:D:335:ASP:N	2.51	0.43
1:E:143:THR:CG2	1:E:144:ILE:N	2.62	0.43
1:E:188:TRP:CZ2	1:E:246:LEU:O	2.71	0.43
1:E:208:HIS:O	1:E:209:ALA:HB2	2.18	0.43
1:E:348:PHE:HE1	1:E:379:TRP:NE1	2.15	0.43
1:D:234:THR:CG2	1:D:235:ALA:N	2.81	0.43
1:B:324:ASN:OD1	1:B:326:ILE:N	2.52	0.43
1:C:55:PHE:CE2	1:C:57:VAL:CG1	3.01	0.43
1:C:188:TRP:CZ2	1:C:246:LEU:O	2.72	0.43
1:D:88:MET:HE2	1:D:88:MET:HB3	1.90	0.43
1:D:152:TRP:HB3	1:D:169:LEU:HD21	2.00	0.43
1:D:324:ASN:OD1	1:D:326:ILE:N	2.52	0.43
1:D:388:VAL:HB	1:D:401:MET:HB2	2.01	0.43
1:E:152:TRP:HB3	1:E:169:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:TRP:HB3	1:E:169:LEU:CD2	2.49	0.43
1:A:234:THR:CG2	1:A:235:ALA:N	2.82	0.43
1:A:280:ILE:HG13	1:A:281:PHE:N	2.32	0.43
1:B:55:PHE:CE2	1:B:57:VAL:CG1	3.02	0.43
1:C:29:ILE:HG21	1:C:88:MET:HE3	2.01	0.43
1:C:346:ILE:HD12	1:C:346:ILE:HA	1.72	0.43
1:D:33:PRO:O	1:D:35:GLU:N	2.51	0.43
1:D:81:PRO:HG3	1:E:54:LEU:HD21	2.00	0.43
1:E:55:PHE:CE2	1:E:57:VAL:CG1	3.01	0.43
1:E:261:GLU:HG2	1:E:286:ARG:N	2.28	0.43
1:A:145:VAL:HG12	1:A:146:PRO:N	2.34	0.43
1:A:208:HIS:O	1:A:209:ALA:HB2	2.18	0.43
1:A:229:TRP:HA	1:A:253:THR:HB	2.01	0.43
1:D:20:LEU:HD23	1:D:143:THR:OG1	2.18	0.43
1:E:148:ALA:O	1:E:149:HIS:HB2	2.19	0.43
1:C:127:ALA:O	1:C:130:PRO:HD2	2.19	0.42
1:E:241:LEU:O	1:E:242:CYS:HB3	2.18	0.42
1:A:22:LEU:HD11	1:A:26:GLN:HB3	2.01	0.42
1:B:10:LYS:O	1:B:11:LEU:C	2.62	0.42
1:B:20:LEU:HD23	1:B:143:THR:OG1	2.19	0.42
1:B:143:THR:CG2	1:B:246:LEU:HD21	2.49	0.42
1:B:202:LEU:HD13	1:B:229:TRP:CZ3	2.54	0.42
1:C:157:PHE:C	1:C:159:GLY:H	2.28	0.42
1:C:246:LEU:HD13	1:C:246:LEU:HA	1.73	0.42
1:D:16:ILE:N	1:D:16:ILE:CD1	2.82	0.42
1:D:55:PHE:CE2	1:D:57:VAL:CG1	3.02	0.42
1:D:131:ALA:O	1:D:132:LEU:C	2.61	0.42
1:D:149:HIS:C	1:D:151:GLY:N	2.76	0.42
1:E:153:ALA:O	1:E:165:ALA:HB1	2.19	0.42
1:E:343:ALA:O	1:E:344:SER:C	2.61	0.42
1:B:7:ASN:O	1:B:8:LEU:C	2.63	0.42
1:B:89:ALA:O	1:B:90:ARG:C	2.62	0.42
1:B:176:ALA:O	1:B:247:PRO:HA	2.19	0.42
1:B:188:TRP:CZ2	1:B:246:LEU:O	2.71	0.42
1:C:356:LEU:HA	1:C:356:LEU:HD23	1.76	0.42
1:D:247:PRO:O	1:D:248:THR:C	2.63	0.42
1:D:343:ALA:O	1:D:344:SER:C	2.62	0.42
1:E:92:PHE:CE2	1:E:98:ARG:HB2	2.55	0.42
1:E:152:TRP:C	1:E:154:ARG:N	2.77	0.42
1:A:30:ALA:HA	1:A:99:LEU:O	2.19	0.42
1:A:67:LYS:HD3	1:B:45:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:HIS:C	1:C:151:GLY:N	2.76	0.42
1:D:80:ALA:HA	1:D:81:PRO:HD3	1.84	0.42
1:D:161:PRO:O	1:D:165:ALA:N	2.52	0.42
1:E:14:LEU:O	1:E:15:ALA:C	2.63	0.42
1:E:152:TRP:CE3	1:E:169:LEU:HD11	2.55	0.42
1:E:245:ASN:HD22	1:E:337:LEU:CD1	2.33	0.42
1:A:77:LEU:H	1:A:77:LEU:CD1	2.33	0.42
1:A:131:ALA:O	1:A:132:LEU:C	2.62	0.42
1:C:18:VAL:HG12	1:C:243:ASN:HD22	1.83	0.42
1:C:88:MET:HE2	1:C:88:MET:HB3	1.90	0.42
1:C:332:VAL:O	1:C:334:PHE:CE2	2.71	0.42
1:D:323:ASP:OD1	1:D:323:ASP:O	2.38	0.42
1:D:352:TYR:HB3	1:D:354:GLU:CG	2.48	0.42
1:E:14:LEU:C	1:E:16:ILE:N	2.77	0.42
1:A:157:PHE:C	1:A:159:GLY:H	2.27	0.42
1:A:220:VAL:O	1:A:220:VAL:HG12	2.19	0.42
1:A:246:LEU:HD13	1:A:246:LEU:HA	1.87	0.42
1:A:280:ILE:HG12	1:A:379:TRP:CZ3	2.55	0.42
1:A:356:LEU:HD12	1:A:365:PHE:CE1	2.54	0.42
1:A:407:VAL:O	1:A:407:VAL:HG12	2.20	0.42
1:B:92:PHE:CE2	1:B:98:ARG:HB2	2.54	0.42
1:C:7:ASN:O	1:C:8:LEU:C	2.62	0.42
1:C:139:VAL:HG23	1:C:140:THR:N	2.34	0.42
1:C:202:LEU:HD13	1:C:229:TRP:CZ3	2.55	0.42
1:D:14:LEU:HD23	1:D:15:ALA:N	2.35	0.42
1:E:80:ALA:HA	1:E:81:PRO:HD3	1.84	0.42
1:E:241:LEU:H	1:E:241:LEU:CD1	2.30	0.42
1:E:247:PRO:O	1:E:248:THR:C	2.63	0.42
1:A:14:LEU:C	1:A:16:ILE:N	2.77	0.42
1:B:320:VAL:HG23	1:B:344:SER:HA	2.01	0.42
1:B:330:GLY:O	1:B:331:LEU:HD23	2.19	0.42
1:B:343:ALA:O	1:B:344:SER:C	2.62	0.42
1:B:348:PHE:HE1	1:B:379:TRP:NE1	2.17	0.42
1:B:402:ARG:O	1:B:403:ARG:C	2.63	0.42
1:C:389:ASP:OD1	1:C:402:ARG:NH2	2.52	0.42
1:D:148:ALA:O	1:D:149:HIS:HB2	2.19	0.42
1:A:202:LEU:HD13	1:A:229:TRP:CZ3	2.55	0.42
1:D:7:ASN:O	1:D:8:LEU:C	2.62	0.42
1:D:210:LEU:HD12	1:D:317:VAL:HG11	2.01	0.42
1:E:74:GLU:C	1:E:76:GLY:N	2.75	0.42
1:E:251:VAL:HG23	1:E:251:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:VAL:HG23	1:A:140:THR:N	2.34	0.42
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.85	0.42
1:B:30:ALA:HA	1:B:99:LEU:O	2.20	0.42
1:C:343:ALA:O	1:C:344:SER:C	2.62	0.42
1:D:195:LEU:O	1:D:197:GLU:N	2.53	0.42
1:D:241:LEU:O	1:D:242:CYS:HB3	2.19	0.42
1:A:77:LEU:C	1:A:79:LYS:N	2.76	0.42
1:A:188:TRP:CZ2	1:A:246:LEU:O	2.73	0.42
1:B:407:VAL:HG12	1:B:407:VAL:O	2.18	0.42
1:C:33:PRO:C	1:C:35:GLU:N	2.77	0.42
1:C:35:GLU:H	1:C:35:GLU:HG2	1.47	0.42
1:C:152:TRP:HB3	1:C:169:LEU:HD21	2.01	0.42
1:D:152:TRP:HB3	1:D:169:LEU:CD2	2.50	0.42
1:D:323:ASP:OD1	1:D:323:ASP:C	2.63	0.42
1:E:127:ALA:O	1:E:130:PRO:HD2	2.20	0.42
1:E:202:LEU:HD13	1:E:229:TRP:CE3	2.55	0.42
1:E:280:ILE:HG13	1:E:281:PHE:N	2.34	0.42
1:E:388:VAL:HB	1:E:401:MET:HB2	2.01	0.42
1:B:264:VAL:HG13	1:B:264:VAL:O	2.19	0.41
1:B:320:VAL:HB	1:B:344:SER:N	2.35	0.41
1:C:14:LEU:C	1:C:16:ILE:N	2.77	0.41
1:C:202:LEU:HD13	1:C:229:TRP:CE3	2.55	0.41
1:C:245:ASN:HD22	1:C:337:LEU:CD1	2.33	0.41
1:D:145:VAL:HG12	1:D:146:PRO:N	2.35	0.41
1:D:407:VAL:O	1:D:407:VAL:HG12	2.20	0.41
1:E:157:PHE:C	1:E:159:GLY:H	2.27	0.41
1:E:352:TYR:HB3	1:E:354:GLU:CG	2.48	0.41
1:A:58:ILE:HD13	1:A:84:LEU:HD11	2.00	0.41
1:A:202:LEU:HD13	1:A:229:TRP:CE3	2.55	0.41
1:A:245:ASN:HD22	1:A:337:LEU:CD1	2.34	0.41
1:B:148:ALA:O	1:B:149:HIS:HB2	2.20	0.41
1:B:167:ARG:O	1:B:170:TRP:NE1	2.54	0.41
1:C:256:HIS:ND1	1:C:369:GLY:HA3	2.35	0.41
1:E:202:LEU:HD13	1:E:229:TRP:CZ3	2.55	0.41
1:E:333:PHE:O	1:E:334:PHE:C	2.62	0.41
1:A:48:TYR:HD1	1:A:52:ALA:O	2.02	0.41
1:C:145:VAL:HG12	1:C:146:PRO:N	2.35	0.41
1:D:10:LYS:O	1:D:11:LEU:C	2.62	0.41
1:D:188:TRP:CZ2	1:D:246:LEU:O	2.72	0.41
1:D:280:ILE:HG13	1:D:281:PHE:N	2.36	0.41
1:B:145:VAL:HG12	1:B:146:PRO:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:LEU:HD12	1:B:169:LEU:O	2.21	0.41
1:B:171:GLU:HA	1:B:174:PHE:CD2	2.56	0.41
1:B:202:LEU:HD13	1:B:229:TRP:CE3	2.56	0.41
1:B:317:VAL:HG22	1:B:346:ILE:HD11	2.03	0.41
1:C:10:LYS:O	1:C:11:LEU:C	2.63	0.41
1:C:272:LEU:HD11	1:C:304:LEU:HD22	2.02	0.41
1:D:293:ARG:HH11	1:D:293:ARG:CB	2.32	0.41
1:A:7:ASN:O	1:A:8:LEU:C	2.64	0.41
1:B:74:GLU:C	1:B:76:GLY:N	2.77	0.41
1:C:48:TYR:HD1	1:C:52:ALA:O	2.03	0.41
1:C:143:THR:HG22	1:C:246:LEU:HD23	2.02	0.41
1:A:33:PRO:C	1:A:35:GLU:N	2.78	0.41
1:A:34:ILE:HD11	1:B:37:VAL:HG13	2.02	0.41
1:A:127:ALA:O	1:A:130:PRO:HD2	2.20	0.41
1:B:77:LEU:H	1:B:77:LEU:CD1	2.33	0.41
1:B:152:TRP:HB3	1:B:169:LEU:HD21	2.02	0.41
1:B:402:ARG:HA	1:B:402:ARG:HD3	1.84	0.41
1:D:14:LEU:O	1:D:15:ALA:C	2.62	0.41
1:D:30:ALA:HA	1:D:99:LEU:O	2.21	0.41
1:D:144:ILE:HG22	1:D:337:LEU:CD2	2.49	0.41
1:D:272:LEU:HD11	1:D:304:LEU:HD22	2.01	0.41
1:E:48:TYR:HD1	1:E:52:ALA:O	2.04	0.41
1:E:389:ASP:OD1	1:E:402:ARG:NH2	2.49	0.41
1:A:152:TRP:C	1:A:154:ARG:N	2.75	0.41
1:A:320:VAL:HG23	1:A:344:SER:HA	2.03	0.41
1:A:389:ASP:OD1	1:A:402:ARG:NH2	2.52	0.41
1:B:33:PRO:C	1:B:35:GLU:N	2.77	0.41
1:B:280:ILE:HG13	1:B:281:PHE:N	2.36	0.41
1:B:333:PHE:O	1:B:334:PHE:C	2.63	0.41
1:C:320:VAL:HG23	1:C:344:SER:HA	2.03	0.41
1:D:33:PRO:C	1:D:35:GLU:N	2.79	0.41
1:A:32:ALA:HA	1:A:33:PRO:HD3	1.82	0.41
1:A:54:LEU:HD21	1:B:81:PRO:HG3	2.03	0.41
1:A:205:ARG:HB2	1:A:207:PHE:CE1	2.56	0.41
1:A:332:VAL:O	1:A:334:PHE:CE2	2.73	0.41
1:B:320:VAL:HB	1:B:343:ALA:HA	2.02	0.41
1:C:131:ALA:O	1:C:132:LEU:C	2.63	0.41
1:C:320:VAL:HB	1:C:344:SER:N	2.35	0.41
1:C:388:VAL:HB	1:C:401:MET:HB2	2.02	0.41
1:D:202:LEU:HD13	1:D:229:TRP:CE3	2.56	0.41
1:D:317:VAL:HG22	1:D:346:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:ASN:OD1	1:E:326:ILE:N	2.54	0.41
1:A:185:ILE:HD12	1:A:185:ILE:N	2.27	0.41
1:A:219:LEU:HD11	1:A:260:VAL:HG12	2.01	0.41
1:B:229:TRP:HA	1:B:253:THR:HB	2.03	0.41
1:C:14:LEU:O	1:C:15:ALA:C	2.63	0.41
1:C:77:LEU:C	1:C:79:LYS:N	2.75	0.41
1:C:392:TYR:HE2	1:D:265:ARG:CD	2.33	0.41
1:D:34:ILE:CD1	1:E:59:TYR:CE2	3.03	0.41
1:D:48:TYR:HD1	1:D:52:ALA:O	2.04	0.41
1:D:77:LEU:H	1:D:77:LEU:CD1	2.33	0.41
1:E:113:PRO:HA	1:E:114:PRO:HD3	1.83	0.41
1:E:219:LEU:HD22	1:E:264:VAL:HB	2.02	0.41
1:A:116:LYS:O	1:A:119:ARG:N	2.54	0.41
1:A:149:HIS:O	1:A:151:GLY:N	2.53	0.41
1:A:161:PRO:O	1:A:165:ALA:N	2.53	0.41
1:A:247:PRO:O	1:A:248:THR:C	2.64	0.41
1:B:113:PRO:HA	1:B:114:PRO:HD3	1.82	0.41
1:B:389:ASP:OD1	1:B:402:ARG:NH2	2.50	0.41
1:C:92:PHE:CE2	1:C:98:ARG:HB2	2.56	0.41
1:C:171:GLU:HA	1:C:174:PHE:CD2	2.55	0.41
1:D:34:ILE:CD1	1:E:59:TYR:HE2	2.33	0.41
1:E:320:VAL:HB	1:E:343:ALA:HA	2.03	0.41
1:B:138:PHE:HB3	1:B:236:THR:CB	2.51	0.40
1:C:320:VAL:HB	1:C:343:ALA:HA	2.03	0.40
1:E:58:ILE:HD11	1:E:84:LEU:HD11	2.03	0.40
1:E:139:VAL:HG23	1:E:140:THR:N	2.36	0.40
1:A:402:ARG:O	1:A:403:ARG:C	2.63	0.40
1:B:219:LEU:HD22	1:B:264:VAL:HB	2.02	0.40
1:C:152:TRP:HB3	1:C:169:LEU:CD2	2.52	0.40
1:D:92:PHE:CE2	1:D:98:ARG:HB2	2.56	0.40
1:E:171:GLU:HA	1:E:174:PHE:CD2	2.55	0.40
1:E:246:LEU:HD13	1:E:246:LEU:HA	1.80	0.40
1:A:29:ILE:HG21	1:A:88:MET:HE3	2.03	0.40
1:A:195:LEU:C	1:A:197:GLU:H	2.30	0.40
1:A:320:VAL:HB	1:A:343:ALA:HA	2.03	0.40
1:B:195:LEU:O	1:B:196:HIS:C	2.65	0.40
1:B:247:PRO:O	1:B:248:THR:C	2.64	0.40
1:C:229:TRP:HA	1:C:253:THR:HB	2.04	0.40
1:D:45:GLU:HB2	1:E:67:LYS:HD3	2.04	0.40
1:E:7:ASN:O	1:E:8:LEU:C	2.63	0.40
1:B:58:ILE:HD11	1:B:84:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TYR:HB3	1:B:354:GLU:CG	2.50	0.40
1:C:311:ALA:O	1:C:348:PHE:HB3	2.22	0.40
1:D:169:LEU:HD12	1:D:169:LEU:O	2.21	0.40
1:D:256:HIS:ND1	1:D:369:GLY:HA3	2.37	0.40
1:D:280:ILE:HG12	1:D:379:TRP:CZ3	2.56	0.40
1:E:140:THR:C	1:E:236:THR:HG21	2.46	0.40
1:E:272:LEU:HD11	1:E:304:LEU:HD22	2.02	0.40
1:E:402:ARG:O	1:E:403:ARG:C	2.64	0.40
1:A:149:HIS:C	1:A:151:GLY:N	2.75	0.40
1:A:320:VAL:HB	1:A:344:SER:N	2.37	0.40
1:D:266:ALA:CB	1:D:280:ILE:HG23	2.47	0.40
1:E:138:PHE:CE2	1:E:234:THR:HG21	2.57	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:D:205:ARG:O	1:E:265:ARG:NH1[3_554]	2.19	0.01

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	391/408 (96%)	316 (81%)	57 (15%)	18 (5%)	2	18
1	B	391/408 (96%)	317 (81%)	56 (14%)	18 (5%)	2	18
1	C	391/408 (96%)	314 (80%)	59 (15%)	18 (5%)	2	18
1	D	391/408 (96%)	315 (81%)	57 (15%)	19 (5%)	1	17
1	E	391/408 (96%)	314 (80%)	59 (15%)	18 (5%)	2	18
All	All	1955/2040 (96%)	1576 (81%)	288 (15%)	91 (5%)	2	18

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ASP
1	A	146	PRO
1	A	148	ALA
1	A	160	LEU
1	A	248	THR
1	B	146	PRO
1	B	148	ALA
1	B	160	LEU
1	B	248	THR
1	C	146	PRO
1	C	148	ALA
1	C	160	LEU
1	C	248	THR
1	D	146	PRO
1	D	148	ALA
1	D	160	LEU
1	D	248	THR
1	E	146	PRO
1	E	148	ALA
1	E	160	LEU
1	E	248	THR
1	A	138	PHE
1	A	237	LYS
1	A	336	THR
1	B	34	ILE
1	B	78	ASP
1	B	237	LYS
1	B	336	THR
1	C	34	ILE
1	C	78	ASP
1	C	138	PHE
1	C	237	LYS
1	C	336	THR
1	D	34	ILE
1	D	78	ASP
1	D	138	PHE
1	D	237	LYS
1	D	336	THR
1	E	34	ILE
1	E	78	ASP
1	E	237	LYS
1	E	336	THR

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Mol	Chain	Res	Type
1	A	34	ILE
1	A	337	LEU
1	B	138	PHE
1	B	337	LEU
1	C	337	LEU
1	D	337	LEU
1	E	138	PHE
1	E	337	LEU
1	A	161	PRO
1	A	196	HIS
1	A	242	CYS
1	B	161	PRO
1	B	196	HIS
1	B	242	CYS
1	B	334	PHE
1	C	161	PRO
1	C	242	CYS
1	D	161	PRO
1	D	242	CYS
1	D	280	ILE
1	D	334	PHE
1	E	161	PRO
1	E	196	HIS
1	E	242	CYS
1	E	280	ILE
1	E	334	PHE
1	A	150	PRO
1	A	280	ILE
1	A	334	PHE
1	B	150	PRO
1	C	150	PRO
1	C	280	ILE
1	D	150	PRO
1	D	185	ILE
1	D	196	HIS
1	E	150	PRO
1	B	280	ILE
1	C	196	HIS
1	C	334	PHE
1	C	113	PRO
1	D	113	PRO
1	A	113	PRO

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Mol	Chain	Res	Type
1	B	113	PRO
1	C	103	GLY
1	E	103	GLY
1	E	113	PRO
1	A	103	GLY
1	B	103	GLY
1	D	103	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	302/312 (97%)	276 (91%)	26 (9%)	10	34
1	B	302/312 (97%)	278 (92%)	24 (8%)	11	37
1	C	302/312 (97%)	278 (92%)	24 (8%)	11	37
1	D	302/312 (97%)	278 (92%)	24 (8%)	11	37
1	E	302/312 (97%)	278 (92%)	24 (8%)	11	37
All	All	1510/1560 (97%)	1388 (92%)	122 (8%)	11	36

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	8	LEU
1	A	14	LEU
1	A	35	GLU
1	A	42	LEU
1	A	63	GLU
1	A	140	THR
1	A	146	PRO
1	A	152	TRP
1	A	167	ARG
1	A	168	ARG
1	A	184	PRO

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Mol	Chain	Res	Type
1	A	185	ILE
1	A	241	LEU
1	A	246	LEU
1	A	265	ARG
1	A	275	THR
1	A	280	ILE
1	A	281	PHE
1	A	293	ARG
1	A	304	LEU
1	A	306	ASP
1	A	344	SER
1	A	354	GLU
1	A	380	MET
1	A	398	THR
1	B	4	PHE
1	B	8	LEU
1	B	14	LEU
1	B	35	GLU
1	B	42	LEU
1	B	63	GLU
1	B	140	THR
1	B	146	PRO
1	B	152	TRP
1	B	167	ARG
1	B	168	ARG
1	B	184	PRO
1	B	185	ILE
1	B	241	LEU
1	B	265	ARG
1	B	275	THR
1	B	280	ILE
1	B	281	PHE
1	B	293	ARG
1	B	304	LEU
1	B	306	ASP
1	B	344	SER
1	B	354	GLU
1	B	398	THR
1	C	4	PHE
1	C	8	LEU
1	C	14	LEU
1	C	35	GLU

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Mol	Chain	Res	Type
1	C	42	LEU
1	C	63	GLU
1	C	140	THR
1	C	146	PRO
1	C	152	TRP
1	C	167	ARG
1	C	168	ARG
1	C	185	ILE
1	C	241	LEU
1	C	246	LEU
1	C	265	ARG
1	C	275	THR
1	C	280	ILE
1	C	281	PHE
1	C	293	ARG
1	C	304	LEU
1	C	306	ASP
1	C	344	SER
1	C	354	GLU
1	C	398	THR
1	D	4	PHE
1	D	8	LEU
1	D	14	LEU
1	D	35	GLU
1	D	42	LEU
1	D	63	GLU
1	D	140	THR
1	D	146	PRO
1	D	152	TRP
1	D	167	ARG
1	D	168	ARG
1	D	185	ILE
1	D	241	LEU
1	D	246	LEU
1	D	265	ARG
1	D	275	THR
1	D	280	ILE
1	D	281	PHE
1	D	293	ARG
1	D	304	LEU
1	D	306	ASP
1	D	344	SER

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Mol	Chain	Res	Type
1	D	354	GLU
1	D	398	THR
1	E	4	PHE
1	E	8	LEU
1	E	14	LEU
1	E	35	GLU
1	E	42	LEU
1	E	63	GLU
1	E	140	THR
1	E	146	PRO
1	E	152	TRP
1	E	167	ARG
1	E	168	ARG
1	E	185	ILE
1	E	241	LEU
1	E	246	LEU
1	E	265	ARG
1	E	275	THR
1	E	280	ILE
1	E	281	PHE
1	E	293	ARG
1	E	304	LEU
1	E	306	ASP
1	E	344	SER
1	E	354	GLU
1	E	398	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	62	GLN
1	A	124	ASN
1	A	192	ASN
1	A	243	ASN
1	A	245	ASN
1	A	345	HIS
1	A	350	GLN
1	A	353	GLN
1	A	355	ASN
1	B	7	ASN
1	B	62	GLN

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Mol	Chain	Res	Type
1	B	124	ASN
1	B	192	ASN
1	B	196	HIS
1	B	227	HIS
1	B	243	ASN
1	B	245	ASN
1	B	350	GLN
1	B	353	GLN
1	B	355	ASN
1	C	7	ASN
1	C	62	GLN
1	C	124	ASN
1	C	192	ASN
1	C	227	HIS
1	C	243	ASN
1	C	245	ASN
1	C	345	HIS
1	C	350	GLN
1	C	353	GLN
1	C	355	ASN
1	D	7	ASN
1	D	62	GLN
1	D	124	ASN
1	D	227	HIS
1	D	245	ASN
1	D	345	HIS
1	D	350	GLN
1	D	353	GLN
1	D	355	ASN
1	E	7	ASN
1	E	62	GLN
1	E	124	ASN
1	E	227	HIS
1	E	245	ASN
1	E	350	GLN
1	E	353	GLN
1	E	355	ASN

5.3.3 RNA ⓘ

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 10 ligands modelled in this entry, 10 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 [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	397/408 (97%)	0.06	3 (0%) 82 60	101, 128, 129, 129	0
1	B	397/408 (97%)	0.25	15 (3%) 44 28	101, 128, 129, 129	0
1	C	397/408 (97%)	0.02	2 (0%) 87 69	101, 128, 129, 129	0
1	D	397/408 (97%)	0.27	22 (5%) 30 20	101, 128, 129, 129	0
1	E	397/408 (97%)	0.15	6 (1%) 72 46	101, 128, 129, 129	0
All	All	1985/2040 (97%)	0.15	48 (2%) 59 37	101, 128, 129, 129	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	333	PHE	5.1
1	B	184	PRO	4.7
1	D	337	LEU	4.3
1	D	186	ALA	4.1
1	B	185	ILE	3.8
1	B	176	ALA	3.6
1	D	239	GLY	3.6
1	B	327	ALA	3.5
1	D	334	PHE	3.5
1	E	408	VAL	2.9
1	E	176	ALA	2.8
1	D	238	GLY	2.8
1	E	184	PRO	2.7
1	B	242	CYS	2.7
1	E	242	CYS	2.7
1	B	334	PHE	2.6
1	D	187	ALA	2.6
1	D	235	ALA	2.6
1	D	336	THR	2.6
1	A	408	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	331	LEU	2.5
1	B	240	ARG	2.5
1	B	127	ALA	2.4
1	D	170	TRP	2.4
1	B	3	ALA	2.4
1	C	3	ALA	2.4
1	D	103	GLY	2.3
1	E	338	PHE	2.3
1	D	247	PRO	2.3
1	D	241	LEU	2.3
1	B	245	ASN	2.3
1	D	320	VAL	2.3
1	D	339	ASP	2.3
1	D	136	THR	2.3
1	D	190	ALA	2.3
1	C	358	GLY	2.3
1	B	408	VAL	2.2
1	D	236	THR	2.2
1	B	248	THR	2.2
1	D	240	ARG	2.1
1	D	185	ILE	2.1
1	B	161	PRO	2.1
1	B	244	PRO	2.1
1	B	241	LEU	2.1
1	E	177	THR	2.1
1	A	184	PRO	2.0
1	A	372	GLU	2.0
1	D	332	VAL	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](#)

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(Å ²)	Q<0.9
2	ZN	E	900	1/1	0.91	0.17	128,128,128,128	0
2	ZN	A	500	1/1	0.92	0.12	128,128,128,128	0
2	ZN	D	800	1/1	0.94	0.16	128,128,128,128	0
2	ZN	A	501	1/1	0.94	0.13	128,128,128,128	0
2	ZN	D	801	1/1	0.95	0.14	128,128,128,128	0
2	ZN	B	600	1/1	0.95	0.11	128,128,128,128	0
2	ZN	B	601	1/1	0.96	0.14	128,128,128,128	0
2	ZN	C	701	1/1	0.97	0.13	128,128,128,128	0
2	ZN	C	700	1/1	0.98	0.13	128,128,128,128	0
2	ZN	E	901	1/1	0.99	0.14	128,128,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.