



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 10:22 pm BST

PDB ID : 169L
Title : PROTEIN FLEXIBILITY AND ADAPTABILITY SEEN IN 25 CRYSTAL FORMS OF T4 LYSOZYME
Authors : Zhang, X.-J.; Matthews, B.W.
Deposited on : 1995-03-24
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

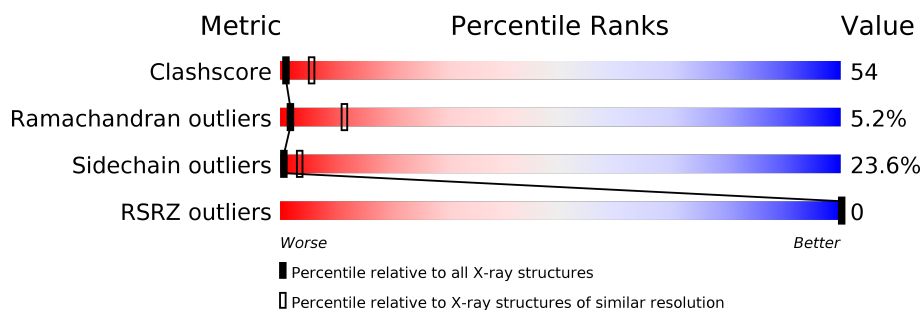
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	164	<div> <div>24%</div> <div>48%</div> <div>25%</div> <div>..</div> </div>
1	B	164	<div> <div>22%</div> <div>58%</div> <div>16%</div> <div>..</div> </div>
1	C	164	<div> <div>20%</div> <div>52%</div> <div>25%</div> <div>..</div> </div>
1	D	164	<div> <div>22%</div> <div>57%</div> <div>16%</div> <div>..</div> </div>
1	E	164	<div> <div>26%</div> <div>51%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6290 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 T4 LYSOZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1258	793	228	230	7			
1	B	162	Total	C	N	O	S	0	0	0
			1258	793	228	230	7			
1	C	162	Total	C	N	O	S	0	0	0
			1258	793	228	230	7			
1	D	162	Total	C	N	O	S	0	0	0
			1258	793	228	230	7			
1	E	162	Total	C	N	O	S	0	0	0
			1258	793	228	230	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	GLU	CONFLICT	UNP P00720
A	131	ALA	VAL	CONFLICT	UNP P00720
A	132	ALA	ASN	CONFLICT	UNP P00720
A	135	ALA	LYS	CONFLICT	UNP P00720
A	136	ALA	SER	CONFLICT	UNP P00720
A	137	ALA	ARG	CONFLICT	UNP P00720
A	139	ALA	TYR	CONFLICT	UNP P00720
A	140	ALA	ASN	CONFLICT	UNP P00720
A	141	ALA	GLN	CONFLICT	UNP P00720
B	128	ALA	GLU	CONFLICT	UNP P00720
B	131	ALA	VAL	CONFLICT	UNP P00720
B	132	ALA	ASN	CONFLICT	UNP P00720
B	135	ALA	LYS	CONFLICT	UNP P00720
B	136	ALA	SER	CONFLICT	UNP P00720
B	137	ALA	ARG	CONFLICT	UNP P00720
B	139	ALA	TYR	CONFLICT	UNP P00720
B	140	ALA	ASN	CONFLICT	UNP P00720
B	141	ALA	GLN	CONFLICT	UNP P00720
C	128	ALA	GLU	CONFLICT	UNP P00720

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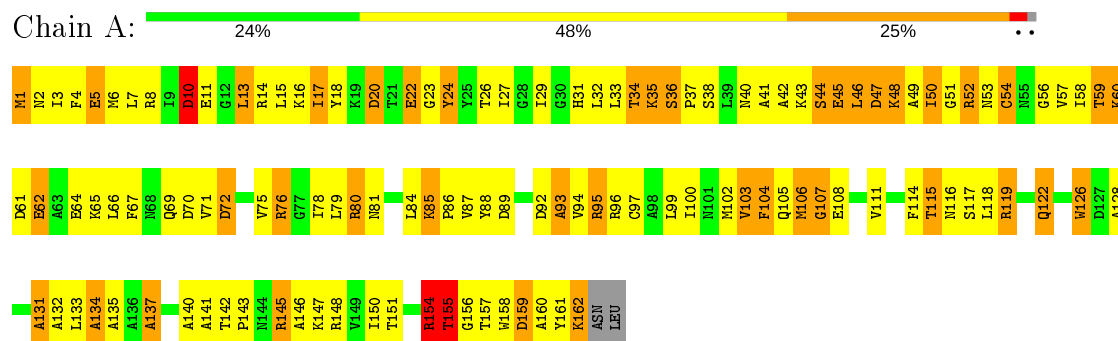
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Chain	Residue	Modelled	Actual	Comment	Reference
C	131	ALA	VAL	CONFLICT	UNP P00720
C	132	ALA	ASN	CONFLICT	UNP P00720
C	135	ALA	LYS	CONFLICT	UNP P00720
C	136	ALA	SER	CONFLICT	UNP P00720
C	137	ALA	ARG	CONFLICT	UNP P00720
C	139	ALA	TYR	CONFLICT	UNP P00720
C	140	ALA	ASN	CONFLICT	UNP P00720
C	141	ALA	GLN	CONFLICT	UNP P00720
D	128	ALA	GLU	CONFLICT	UNP P00720
D	131	ALA	VAL	CONFLICT	UNP P00720
D	132	ALA	ASN	CONFLICT	UNP P00720
D	135	ALA	LYS	CONFLICT	UNP P00720
D	136	ALA	SER	CONFLICT	UNP P00720
D	137	ALA	ARG	CONFLICT	UNP P00720
D	139	ALA	TYR	CONFLICT	UNP P00720
D	140	ALA	ASN	CONFLICT	UNP P00720
D	141	ALA	GLN	CONFLICT	UNP P00720
E	128	ALA	GLU	CONFLICT	UNP P00720
E	131	ALA	VAL	CONFLICT	UNP P00720
E	132	ALA	ASN	CONFLICT	UNP P00720
E	135	ALA	LYS	CONFLICT	UNP P00720
E	136	ALA	SER	CONFLICT	UNP P00720
E	137	ALA	ARG	CONFLICT	UNP P00720
E	139	ALA	TYR	CONFLICT	UNP P00720
E	140	ALA	ASN	CONFLICT	UNP P00720
E	141	ALA	GLN	CONFLICT	UNP P00720

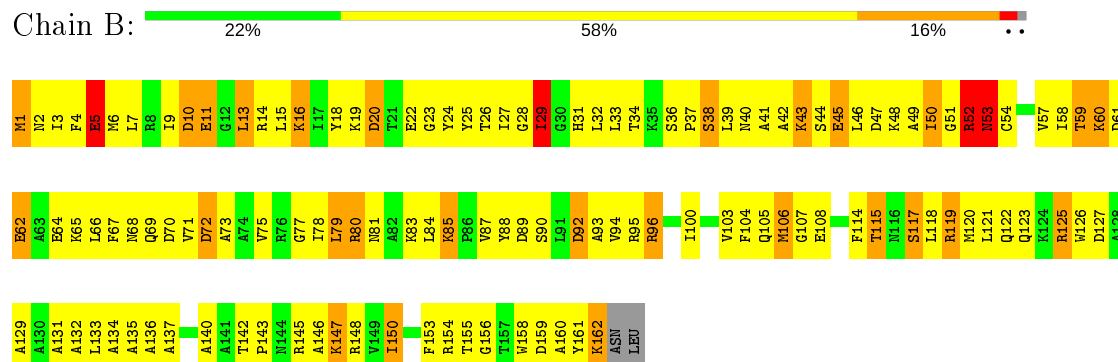
3 Residue-property plots

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

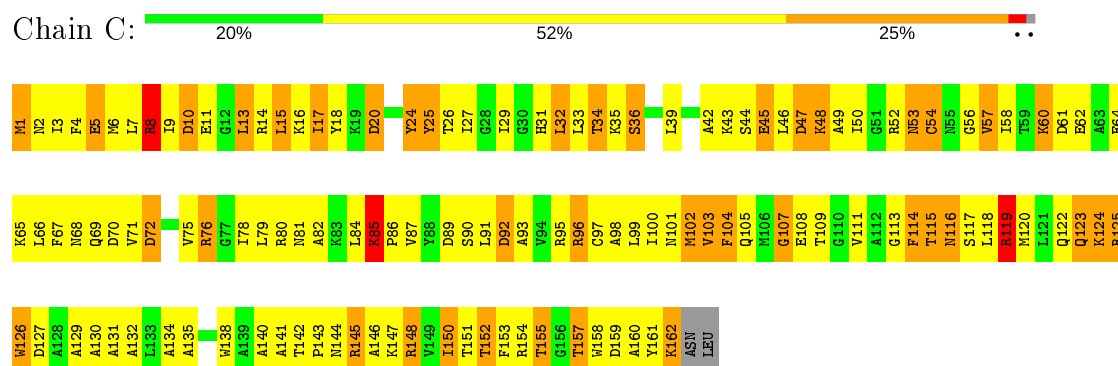
• Molecule 1: T4 LYSOZYME



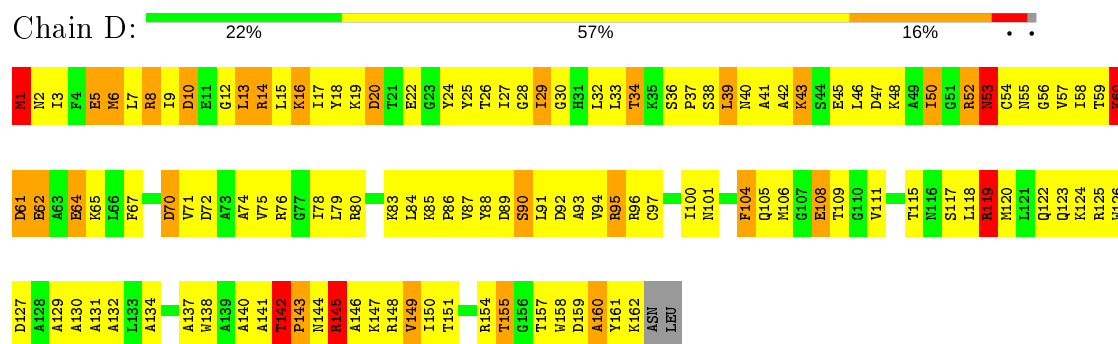
• Molecule 1: T4 LYSOZYME



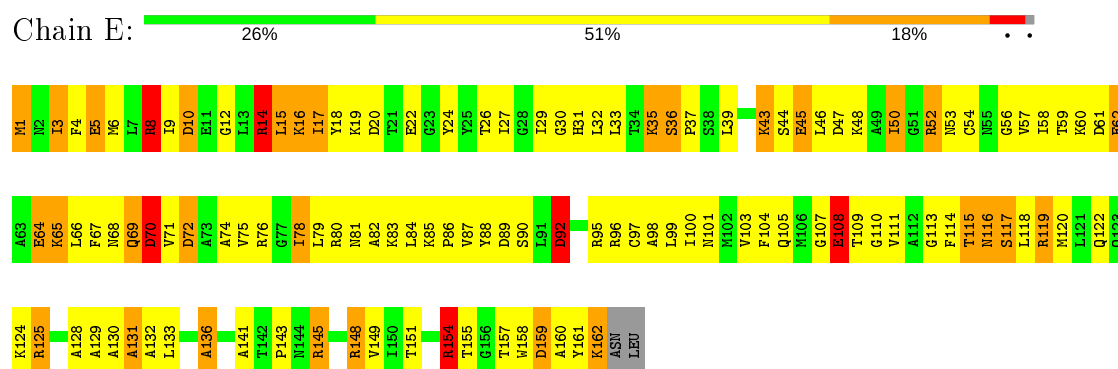
• Molecule 1: T4 LYSOZYME



• Molecule 1: T4 LYSOZYME



• Molecule 1: T4 LYSOZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.40 Å 112.30 Å 135.20 Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00 51.85 – 2.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-3.00) 59.9 (51.85-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 2.96 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.161 , (Not available) 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 115.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6290	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.94	5/1277 (0.4%)	1.50	20/1722 (1.2%)
1	B	0.97	7/1277 (0.5%)	1.44	15/1722 (0.9%)
1	C	0.92	5/1277 (0.4%)	1.53	23/1722 (1.3%)
1	D	0.96	5/1277 (0.4%)	1.55	23/1722 (1.3%)
1	E	0.96	6/1277 (0.5%)	1.49	22/1722 (1.3%)
All	All	0.95	28/6385 (0.4%)	1.50	103/8610 (1.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	GLU	CD-OE2	7.50	1.33	1.25
1	E	5	GLU	CD-OE2	7.22	1.33	1.25
1	D	108	GLU	CD-OE2	7.21	1.33	1.25
1	D	62	GLU	CD-OE2	7.05	1.33	1.25
1	B	62	GLU	CD-OE2	6.93	1.33	1.25
1	A	22	GLU	CD-OE2	6.86	1.33	1.25
1	E	64	GLU	CD-OE2	6.72	1.33	1.25
1	A	45	GLU	CD-OE2	6.61	1.32	1.25
1	E	62	GLU	CD-OE2	6.60	1.32	1.25
1	A	5	GLU	CD-OE2	6.38	1.32	1.25
1	C	45	GLU	CD-OE2	6.36	1.32	1.25
1	E	45	GLU	CD-OE2	6.26	1.32	1.25
1	A	62	GLU	CD-OE2	6.19	1.32	1.25
1	D	64	GLU	CD-OE2	6.15	1.32	1.25
1	B	64	GLU	CD-OE2	6.10	1.32	1.25
1	E	22	GLU	CD-OE2	6.09	1.32	1.25
1	D	5	GLU	CD-OE2	6.05	1.32	1.25
1	D	45	GLU	CD-OE2	5.92	1.32	1.25
1	B	11	GLU	CD-OE2	5.92	1.32	1.25
1	A	108	GLU	CD-OE2	5.71	1.31	1.25
1	C	64	GLU	CD-OE2	5.59	1.31	1.25
1	B	153	PHE	CE1-CZ	5.51	1.47	1.37
1	E	108	GLU	CD-OE2	5.40	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	GLU	CD-OE2	5.34	1.31	1.25
1	B	5	GLU	CD-OE2	5.27	1.31	1.25
1	C	5	GLU	CD-OE2	5.23	1.31	1.25
1	C	108	GLU	CD-OE2	5.21	1.31	1.25
1	B	108	GLU	CD-OE2	5.17	1.31	1.25

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	THR	C-N-CD	-12.14	93.88	120.60
1	C	119	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	D	159	ASP	CB-CG-OD2	-10.16	109.15	118.30
1	A	92	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	A	20	ASP	CB-CG-OD2	-9.13	110.09	118.30
1	E	70	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	A	61	ASP	CB-CG-OD1	8.97	126.37	118.30
1	B	52	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	C	10	ASP	CB-CG-OD1	8.69	126.12	118.30
1	D	61	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	E	148	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	52	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	E	70	ASP	CB-CG-OD1	7.62	125.16	118.30
1	E	72	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	C	20	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	10	ASP	CB-CG-OD1	7.50	125.05	118.30
1	C	70	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	20	ASP	CB-CG-OD1	7.45	125.00	118.30
1	D	10	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	A	61	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	C	8	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	20	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	154	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	E	10	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	154	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	159	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	89	ASP	CB-CG-OD1	6.85	124.46	118.30
1	E	92	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	47	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	E	72	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	10	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	D	70	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	154	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	E	95	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	D	145	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	47	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	8	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	C	47	ASP	CB-CG-OD1	6.52	124.17	118.30
1	E	80	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	47	ASP	CB-CG-OD1	6.44	124.10	118.30
1	B	153	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	B	95	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	C	10	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	A	70	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	E	20	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	D	95	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	119	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	80	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	76	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	B	153	PHE	CB-CG-CD1	6.14	125.10	120.80
1	D	127	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	61	ASP	CB-CG-OD1	6.08	123.77	118.30
1	D	125	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	61	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	C	48	LYS	CB-CA-C	-6.05	98.31	110.40
1	D	70	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	72	ASP	CB-CG-OD1	5.99	123.69	118.30
1	E	95	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	20	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	20	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	125	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	89	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	D	1	MET	CA-C-N	-5.81	104.42	117.20
1	A	76	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	E	47	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	159	ASP	CB-CG-OD1	5.77	123.50	118.30
1	D	20	ASP	CB-CG-OD1	5.75	123.48	118.30
1	A	47	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	E	125	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	20	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	61	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	24	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	C	72	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	47	ASP	CB-CG-OD1	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	TYR	CB-CG-CD1	-5.54	117.67	121.00
1	C	92	ASP	CB-CG-OD1	5.54	123.29	118.30
1	E	61	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	14	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	145	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	89	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	E	14	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	72	ASP	CB-CG-OD1	5.37	123.13	118.30
1	E	8	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	4	PHE	CB-CG-CD1	5.34	124.54	120.80
1	C	125	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	76	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	25	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	A	80	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	10	ASP	CB-CG-OD1	5.26	123.03	118.30
1	E	159	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	E	10	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	8	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	E	154	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	119	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	D	8	ARG	CG-CD-NE	5.15	122.61	111.80
1	E	61	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	57	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	E	59	THR	CA-CB-CG2	-5.14	105.20	112.40
1	E	154	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	A	80	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	80	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	80	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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	1258	0	1287	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1258	0	1287	162	0
1	C	1258	0	1287	145	0
1	D	1258	0	1287	130	0
1	E	1258	0	1287	107	0
All	All	6290	0	6435	688	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (688) 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:D:50:ILE:HD13	1:D:62:GLU:HG2	1.31	1.11
1:A:13:LEU:HD21	1:A:15:LEU:HD21	1.32	1.11
1:B:50:ILE:HD11	1:B:52:ARG:HG2	1.17	1.10
1:A:87:VAL:HG22	1:A:122:GLN:HG3	1.33	1.10
1:A:116:ASN:HA	1:A:119:ARG:HD3	1.38	1.05
1:D:53:ASN:ND2	1:D:53:ASN:H	1.52	1.04
1:D:53:ASN:HD22	1:D:53:ASN:N	1.55	1.02
1:C:120:MET:HE1	1:C:129:ALA:HA	1.41	0.99
1:B:79:LEU:HA	1:B:85:LYS:HG3	1.42	0.99
1:D:120:MET:HE3	1:D:129:ALA:HA	1.48	0.94
1:A:81:ASN:ND2	1:A:84:LEU:HD12	1.83	0.94
1:A:16:LYS:HB2	1:A:57:VAL:HG22	1.49	0.93
1:A:72:ASP:HB3	1:A:76:ARG:NH2	1.82	0.93
1:B:120:MET:HE1	1:B:129:ALA:HA	1.47	0.93
1:C:53:ASN:H	1:C:53:ASN:ND2	1.67	0.91
1:A:1:MET:CE	1:A:5:GLU:HB3	2.00	0.91
1:B:120:MET:CE	1:B:129:ALA:HA	2.01	0.90
1:C:120:MET:CE	1:C:129:ALA:HA	2.03	0.89
1:D:79:LEU:HA	1:D:85:LYS:HG3	1.54	0.89
1:B:53:ASN:ND2	1:B:53:ASN:H	1.70	0.88
1:C:53:ASN:H	1:C:53:ASN:HD22	0.88	0.87
1:E:1:MET:HB3	1:E:158:TRP:CD2	2.09	0.87
1:A:52:ARG:NH1	1:A:54:CYS:HA	1.90	0.87
1:E:1:MET:HE3	1:E:5:GLU:HB3	1.56	0.86
1:D:50:ILE:HD13	1:D:62:GLU:CG	2.06	0.84
1:E:116:ASN:HA	1:E:119:ARG:HD3	1.59	0.84
1:C:53:ASN:N	1:C:53:ASN:HD22	1.71	0.84
1:A:103:VAL:HG23	1:A:111:VAL:HG21	1.60	0.84
1:D:14:ARG:HG3	1:D:18:TYR:CE2	2.12	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HB3	1:C:158:TRP:CD2	2.14	0.83
1:D:8:ARG:HH21	1:D:9:ILE:HD11	1.43	0.83
1:A:94:VAL:HG22	1:A:158:TRP:CZ2	2.13	0.83
1:A:79:LEU:HA	1:A:85:LYS:HG3	1.61	0.83
1:A:103:VAL:CG2	1:A:111:VAL:HG21	2.10	0.82
1:A:87:VAL:CG2	1:A:122:GLN:HG3	2.09	0.82
1:A:116:ASN:HA	1:A:119:ARG:CD	2.09	0.82
1:A:145:ARG:HA	1:A:148:ARG:NH2	1.95	0.81
1:B:1:MET:HB3	1:B:158:TRP:CD2	2.15	0.81
1:B:105:GLN:NE2	1:B:145:ARG:HH11	1.79	0.81
1:B:59:THR:HG23	1:B:62:GLU:CD	2.01	0.81
1:B:39:LEU:HD11	1:B:43:LYS:HD2	1.63	0.81
1:D:119:ARG:O	1:D:123:GLN:HG2	1.80	0.81
1:D:1:MET:CE	1:D:5:GLU:HB3	2.11	0.81
1:C:72:ASP:HB3	1:C:76:ARG:NH2	1.95	0.80
1:E:4:PHE:CE1	1:E:29:ILE:HD11	2.16	0.80
1:B:50:ILE:HG13	1:B:51:GLY:N	1.96	0.80
1:A:24:TYR:CD1	1:A:35:LYS:HB3	2.17	0.80
1:C:146:ALA:O	1:C:150:ILE:HG13	1.82	0.80
1:C:148:ARG:HG2	1:C:160:ALA:HB1	1.64	0.80
1:D:151:THR:O	1:D:155:THR:HG23	1.82	0.79
1:E:155:THR:O	1:E:157:THR:HG23	1.81	0.79
1:E:92:ASP:O	1:E:96:ARG:HG3	1.83	0.79
1:A:105:GLN:HB2	1:A:145:ARG:NH1	1.99	0.78
1:D:14:ARG:O	1:D:15:LEU:HD23	1.83	0.78
1:C:20:ASP:OD2	1:C:24:TYR:HB2	1.83	0.78
1:A:24:TYR:CE1	1:A:35:LYS:HB3	2.18	0.78
1:B:53:ASN:HD22	1:B:53:ASN:H	1.31	0.78
1:D:100:ILE:O	1:D:104:PHE:HB2	1.84	0.78
1:C:87:VAL:HG22	1:C:122:GLN:HG3	1.67	0.77
1:B:1:MET:CE	1:B:5:GLU:HB3	2.14	0.77
1:E:120:MET:HE3	1:E:129:ALA:HA	1.65	0.76
1:C:1:MET:HE2	1:C:5:GLU:HB3	1.67	0.76
1:B:65:LYS:O	1:B:69:GLN:HG3	1.85	0.76
1:E:1:MET:CE	1:E:5:GLU:HB3	2.16	0.76
1:E:120:MET:HE3	1:E:129:ALA:CA	2.16	0.76
1:B:15:LEU:O	1:B:27:ILE:HD11	1.86	0.75
1:A:35:LYS:HD3	1:E:79:LEU:HD11	1.68	0.75
1:A:1:MET:HE2	1:A:5:GLU:HB3	1.68	0.75
1:D:6:MET:HG3	1:D:158:TRP:HZ3	1.51	0.74
1:A:59:THR:HG23	1:A:62:GLU:CD	2.08	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HD2	1:B:161:TYR:CE2	2.22	0.74
1:D:1:MET:HE2	1:D:5:GLU:HB3	1.67	0.74
1:A:107:GLY:O	1:A:111:VAL:HG23	1.86	0.74
1:B:148:ARG:HB3	1:B:161:TYR:CZ	2.23	0.74
1:B:50:ILE:CD1	1:B:52:ARG:HG2	2.10	0.74
1:A:1:MET:HE3	1:A:5:GLU:HB3	1.69	0.74
1:E:15:LEU:N	1:E:15:LEU:HD23	2.03	0.74
1:B:32:LEU:HD23	1:B:33:LEU:N	2.03	0.74
1:D:8:ARG:NH2	1:D:9:ILE:HD11	2.02	0.74
1:A:13:LEU:HD21	1:A:15:LEU:CD2	2.16	0.74
1:B:120:MET:HE1	1:B:132:ALA:HB3	1.70	0.74
1:C:1:MET:CE	1:C:5:GLU:HB3	2.18	0.74
1:D:6:MET:HG3	1:D:158:TRP:CZ3	2.22	0.73
1:C:1:MET:HB3	1:C:158:TRP:CE2	2.23	0.73
1:E:128:ALA:O	1:E:131:ALA:HB3	1.88	0.73
1:C:24:TYR:CD1	1:C:35:LYS:HB3	2.24	0.73
1:D:130:ALA:CB	1:D:154:ARG:HG3	2.17	0.73
1:B:5:GLU:O	1:B:9:ILE:HD12	1.87	0.73
1:A:16:LYS:CB	1:A:57:VAL:HG22	2.17	0.73
1:B:59:THR:HG23	1:B:62:GLU:OE1	1.88	0.73
1:E:24:TYR:CE1	1:E:35:LYS:HB3	2.24	0.73
1:C:162:LYS:HB3	1:C:162:LYS:NZ	2.04	0.72
1:D:130:ALA:HB2	1:D:154:ARG:HG3	1.72	0.72
1:A:81:ASN:O	1:A:85:LYS:HB2	1.89	0.72
1:E:87:VAL:HG21	1:E:118:LEU:HB3	1.70	0.72
1:B:105:GLN:HE21	1:B:145:ARG:HH11	1.36	0.72
1:B:75:VAL:CG2	1:B:100:ILE:HD11	2.20	0.72
1:A:60:LYS:HD2	1:A:60:LYS:O	1.89	0.72
1:B:146:ALA:O	1:B:150:ILE:HG13	1.90	0.72
1:E:39:LEU:HD12	1:E:39:LEU:O	1.90	0.71
1:C:100:ILE:O	1:C:104:PHE:HB2	1.90	0.71
1:C:3:ILE:HG12	1:C:67:PHE:HZ	1.55	0.71
1:C:114:PHE:HB3	1:C:117:SER:HB2	1.73	0.71
1:A:105:GLN:HB2	1:A:145:ARG:HH12	1.55	0.71
1:C:159:ASP:HA	1:C:162:LYS:HE2	1.72	0.71
1:B:120:MET:CB	1:B:129:ALA:HB2	2.21	0.70
1:A:88:TYR:O	1:A:96:ARG:NE	2.25	0.70
1:B:1:MET:HB3	1:B:158:TRP:CG	2.26	0.70
1:B:1:MET:HE3	1:B:5:GLU:HG3	1.74	0.70
1:A:87:VAL:HG22	1:A:122:GLN:CG	2.19	0.70
1:D:38:SER:HB3	1:D:41:ALA:HB2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LYS:NZ	1:A:89:ASP:OD2	2.25	0.69
1:B:105:GLN:HB2	1:B:145:ARG:NH1	2.07	0.69
1:B:105:GLN:HB2	1:B:145:ARG:CZ	2.22	0.69
1:D:87:VAL:HG11	1:D:118:LEU:HD23	1.73	0.69
1:C:76:ARG:O	1:C:80:ARG:HD3	1.92	0.69
1:B:38:SER:HG	1:B:41:ALA:H	1.41	0.69
1:E:130:ALA:HB2	1:E:154:ARG:HG3	1.74	0.69
1:E:100:ILE:O	1:E:103:VAL:HG12	1.92	0.69
1:D:1:MET:HB3	1:D:158:TRP:CD2	2.28	0.68
1:A:78:ILE:HG23	1:A:84:LEU:HB3	1.74	0.68
1:C:45:GLU:O	1:C:48:LYS:HB2	1.93	0.68
1:D:61:ASP:O	1:D:64:GLU:N	2.23	0.68
1:B:159:ASP:HA	1:B:162:LYS:HG2	1.74	0.68
1:B:13:LEU:HD12	1:B:29:ILE:HG12	1.76	0.68
1:C:9:ILE:HG21	1:C:161:TYR:HD2	1.58	0.68
1:B:120:MET:HB3	1:B:129:ALA:HB2	1.76	0.68
1:E:31:HIS:CD2	1:E:66:LEU:HD22	2.28	0.68
1:E:8:ARG:NH2	1:E:9:ILE:HG13	2.09	0.68
1:C:52:ARG:HG3	1:C:53:ASN:N	2.09	0.67
1:E:33:LEU:HD11	1:E:46:LEU:HB2	1.77	0.67
1:A:115:THR:HG22	1:A:119:ARG:HD2	1.75	0.67
1:B:155:THR:OG1	1:B:156:GLY:N	2.26	0.67
1:A:155:THR:OG1	1:A:157:THR:N	2.27	0.67
1:E:74:ALA:O	1:E:78:ILE:HD12	1.94	0.67
1:C:102:MET:HE3	1:C:111:VAL:HG13	1.76	0.67
1:B:50:ILE:HG12	1:B:54:CYS:SG	2.35	0.66
1:B:59:THR:N	1:B:62:GLU:OE1	2.28	0.66
1:C:151:THR:O	1:C:155:THR:HG23	1.96	0.66
1:A:103:VAL:O	1:A:107:GLY:N	2.28	0.66
1:B:1:MET:HE2	1:B:5:GLU:HB3	1.75	0.66
1:B:38:SER:OG	1:B:40:ASN:N	2.29	0.66
1:B:2:ASN:OD1	1:B:5:GLU:HB2	1.96	0.66
1:B:120:MET:CE	1:B:132:ALA:HB3	2.24	0.65
1:B:105:GLN:NE2	1:B:145:ARG:NH1	2.43	0.65
1:E:1:MET:HB3	1:E:158:TRP:CG	2.31	0.65
1:B:125:ARG:O	1:B:127:ASP:N	2.29	0.65
1:B:50:ILE:HD11	1:B:52:ARG:CG	2.11	0.65
1:B:81:ASN:HB3	1:B:84:LEU:HB2	1.78	0.65
1:A:33:LEU:HD11	1:A:46:LEU:HD13	1.77	0.65
1:A:3:ILE:HD13	1:A:71:VAL:HG21	1.77	0.65
1:C:50:ILE:HD11	1:C:52:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:TRP:O	1:C:141:ALA:HB3	1.96	0.65
1:B:118:LEU:O	1:B:121:LEU:N	2.30	0.65
1:A:115:THR:HG22	1:A:116:ASN:N	2.11	0.64
1:E:26:THR:HG22	1:E:27:ILE:N	2.11	0.64
1:A:20:ASP:OD1	1:A:23:GLY:N	2.29	0.64
1:D:88:TYR:HE2	1:D:100:ILE:HD11	1.62	0.64
1:B:39:LEU:O	1:B:39:LEU:HD12	1.98	0.64
1:C:13:LEU:HD21	1:C:15:LEU:HD21	1.80	0.64
1:D:3:ILE:HG12	1:D:67:PHE:HZ	1.62	0.64
1:A:96:ARG:O	1:A:100:ILE:HD12	1.98	0.63
1:C:17:ILE:HD12	1:C:56:GLY:HA2	1.79	0.63
1:B:75:VAL:HG22	1:B:100:ILE:HD11	1.79	0.63
1:E:81:ASN:OD1	1:E:83:LYS:N	2.31	0.63
1:A:159:ASP:HA	1:A:162:LYS:HE2	1.80	0.63
1:A:2:ASN:OD1	1:A:5:GLU:HB2	1.98	0.63
1:B:79:LEU:CA	1:B:85:LYS:HG3	2.24	0.63
1:D:60:LYS:NZ	1:D:60:LYS:O	2.28	0.63
1:E:4:PHE:HA	1:E:67:PHE:CE2	2.33	0.63
1:B:44:SER:O	1:B:48:LYS:HG3	1.98	0.63
1:C:26:THR:HG22	1:C:27:ILE:H	1.62	0.63
1:D:142:THR:O	1:D:144:ASN:N	2.31	0.63
1:A:159:ASP:OD1	1:A:162:LYS:HE2	1.98	0.62
1:A:47:ASP:O	1:A:51:GLY:N	2.30	0.62
1:D:142:THR:N	1:D:143:PRO:HD3	2.14	0.62
1:E:33:LEU:CD1	1:E:46:LEU:HB2	2.29	0.62
1:A:94:VAL:HG22	1:A:158:TRP:CE2	2.34	0.62
1:B:19:LYS:HA	1:B:24:TYR:O	1.99	0.62
1:A:158:TRP:O	1:A:162:LYS:HG2	1.98	0.62
1:A:71:VAL:HG12	1:A:72:ASP:N	2.14	0.62
1:C:1:MET:HB3	1:C:158:TRP:CG	2.34	0.62
1:E:50:ILE:HD13	1:E:62:GLU:OE1	2.00	0.62
1:A:155:THR:OG1	1:A:156:GLY:N	2.28	0.62
1:A:35:LYS:HD3	1:E:79:LEU:CD1	2.30	0.62
1:B:79:LEU:HD13	1:C:35:LYS:HD2	1.79	0.62
1:D:92:ASP:O	1:D:96:ARG:HG3	2.00	0.62
1:B:158:TRP:O	1:B:162:LYS:HG2	2.00	0.61
1:C:26:THR:HG22	1:C:27:ILE:N	2.15	0.61
1:B:38:SER:OG	1:B:39:LEU:N	2.32	0.61
1:A:27:ILE:O	1:A:31:HIS:HB3	2.00	0.61
1:B:93:ALA:HA	1:B:96:ARG:HG3	1.82	0.61
1:A:32:LEU:HD23	1:A:32:LEU:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ASP:HB3	1:D:145:ARG:HG3	1.81	0.61
1:A:59:THR:HG23	1:A:62:GLU:OE1	2.01	0.61
1:B:87:VAL:HG21	1:B:118:LEU:HB3	1.82	0.61
1:C:50:ILE:HG22	1:C:66:LEU:HD21	1.81	0.61
1:B:140:ALA:O	1:B:143:PRO:HD3	2.01	0.61
1:B:1:MET:HE3	1:B:5:GLU:HB3	1.83	0.61
1:D:50:ILE:O	1:D:50:ILE:HD12	2.01	0.61
1:A:146:ALA:O	1:A:150:ILE:HG13	2.01	0.60
1:C:1:MET:HG3	1:C:2:ASN:H	1.65	0.60
1:C:85:LYS:N	1:C:86:PRO:HD2	2.14	0.60
1:A:36:SER:O	1:A:38:SER:N	2.33	0.60
1:C:103:VAL:O	1:C:107:GLY:N	2.34	0.60
1:C:158:TRP:O	1:C:162:LYS:NZ	2.33	0.60
1:E:116:ASN:O	1:E:120:MET:HG3	2.02	0.60
1:E:71:VAL:O	1:E:75:VAL:HG23	2.02	0.60
1:A:52:ARG:HH12	1:A:54:CYS:HA	1.66	0.60
1:B:137:ALA:O	1:B:140:ALA:N	2.35	0.60
1:C:81:ASN:OD1	1:C:82:ALA:N	2.34	0.60
1:C:116:ASN:HA	1:C:119:ARG:HD3	1.83	0.60
1:D:117:SER:HA	1:D:120:MET:HE2	1.83	0.60
1:D:8:ARG:CZ	1:D:9:ILE:HG13	2.31	0.60
1:E:120:MET:CE	1:E:129:ALA:HA	2.30	0.60
1:E:44:SER:OG	1:E:45:GLU:N	2.32	0.60
1:B:159:ASP:HA	1:B:162:LYS:CG	2.32	0.59
1:C:7:LEU:HD22	1:C:11:GLU:HG2	1.82	0.59
1:B:123:GLN:HB2	1:B:125:ARG:HD3	1.83	0.59
1:A:87:VAL:HA	1:A:122:GLN:HG3	1.83	0.59
1:B:94:VAL:HG22	1:B:158:TRP:CZ2	2.37	0.59
1:D:124:LYS:HA	1:D:126:TRP:CZ3	2.37	0.59
1:D:46:LEU:O	1:D:50:ILE:HG23	2.02	0.59
1:B:88:TYR:CE1	1:B:96:ARG:HB3	2.37	0.59
1:D:87:VAL:HG22	1:D:122:GLN:NE2	2.18	0.59
1:A:5:GLU:HA	1:A:5:GLU:OE1	2.03	0.59
1:A:88:TYR:CZ	1:A:96:ARG:HD2	2.37	0.59
1:E:98:ALA:HB1	1:E:149:VAL:HG13	1.84	0.58
1:D:93:ALA:HB2	1:E:19:LYS:NZ	2.18	0.58
1:A:137:ALA:O	1:A:140:ALA:HB3	2.03	0.58
1:C:32:LEU:O	1:C:32:LEU:HD23	2.01	0.58
1:C:81:ASN:O	1:C:85:LYS:HB2	2.04	0.58
1:D:124:LYS:HG2	1:D:126:TRP:CH2	2.38	0.58
1:E:32:LEU:C	1:E:32:LEU:HD23	2.24	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ASP:O	1:B:23:GLY:N	2.36	0.58
1:A:45:GLU:HA	1:A:45:GLU:OE1	2.02	0.58
1:C:75:VAL:O	1:C:78:ILE:N	2.37	0.58
1:C:71:VAL:HG11	1:D:36:SER:HB2	1.85	0.58
1:C:78:ILE:O	1:C:81:ASN:N	2.34	0.58
1:E:39:LEU:HD11	1:E:43:LYS:HD2	1.86	0.57
1:E:50:ILE:HD13	1:E:62:GLU:CD	2.25	0.57
1:D:87:VAL:HG22	1:D:122:GLN:HE21	1.69	0.57
1:E:81:ASN:O	1:E:85:LYS:HB2	2.03	0.57
1:B:59:THR:O	1:B:62:GLU:HB2	2.04	0.57
1:C:141:ALA:C	1:C:143:PRO:HD3	2.24	0.57
1:D:13:LEU:HD12	1:D:28:GLY:HA2	1.85	0.57
1:A:71:VAL:HG11	1:B:36:SER:HB2	1.85	0.57
1:B:51:GLY:O	1:B:52:ARG:HB3	2.03	0.57
1:B:159:ASP:CA	1:B:162:LYS:HG2	2.35	0.57
1:D:141:ALA:C	1:D:143:PRO:HD3	2.24	0.57
1:B:120:MET:HB2	1:B:129:ALA:HB2	1.86	0.57
1:C:15:LEU:HB3	1:C:58:ILE:HG13	1.87	0.57
1:D:58:ILE:HG22	1:D:62:GLU:OE1	2.04	0.57
1:D:1:MET:HE3	1:D:5:GLU:HB3	1.84	0.56
1:B:119:ARG:O	1:B:123:GLN:HG2	2.05	0.56
1:B:46:LEU:O	1:B:49:ALA:HB3	2.05	0.56
1:C:124:LYS:HA	1:C:126:TRP:CZ3	2.41	0.56
1:D:16:LYS:HG3	1:D:57:VAL:HG22	1.87	0.56
1:D:16:LYS:HA	1:D:56:GLY:O	2.05	0.56
1:E:120:MET:HE3	1:E:129:ALA:N	2.19	0.56
1:B:50:ILE:HG13	1:B:51:GLY:H	1.68	0.56
1:B:6:MET:CE	1:B:158:TRP:HZ3	2.17	0.56
1:A:64:GLU:O	1:A:67:PHE:HB3	2.05	0.56
1:A:65:LYS:NZ	1:A:69:GLN:OE1	2.29	0.56
1:C:84:LEU:C	1:C:86:PRO:HD2	2.26	0.56
1:B:105:GLN:HB2	1:B:145:ARG:NH2	2.21	0.56
1:B:45:GLU:OE1	1:B:45:GLU:HA	2.00	0.56
1:D:64:GLU:O	1:D:67:PHE:HB3	2.05	0.56
1:E:159:ASP:OD1	1:E:162:LYS:HD2	2.04	0.56
1:D:1:MET:HB3	1:D:158:TRP:CG	2.41	0.56
1:D:71:VAL:O	1:D:75:VAL:HG23	2.05	0.56
1:E:4:PHE:HB2	1:E:67:PHE:CD2	2.41	0.56
1:A:95:ARG:HD2	1:A:126:TRP:CH2	2.40	0.55
1:C:75:VAL:HG12	1:C:79:LEU:HD12	1.88	0.55
1:C:132:ALA:O	1:C:135:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:LEU:HD21	1:E:111:VAL:HG12	1.87	0.55
1:D:84:LEU:HD12	1:D:108:GLU:HG2	1.89	0.55
1:E:151:THR:HG21	1:E:160:ALA:HB2	1.87	0.55
1:B:59:THR:H	1:B:62:GLU:HB2	1.72	0.55
1:C:24:TYR:HB3	1:C:32:LEU:HD12	1.87	0.55
1:D:67:PHE:O	1:D:71:VAL:HG23	2.06	0.55
1:B:75:VAL:HG21	1:C:36:SER:HB2	1.87	0.55
1:D:85:LYS:N	1:D:86:PRO:HD2	2.22	0.55
1:E:158:TRP:O	1:E:162:LYS:HG2	2.07	0.55
1:D:117:SER:HA	1:D:120:MET:CE	2.37	0.55
1:D:79:LEU:HD13	1:E:35:LYS:HD2	1.87	0.55
1:D:8:ARG:HH21	1:D:9:ILE:CD1	2.16	0.55
1:A:95:ARG:NH2	1:A:155:THR:O	2.39	0.54
1:A:14:ARG:HG3	1:A:18:TYR:CE1	2.42	0.54
1:B:16:LYS:HG3	1:B:57:VAL:HG22	1.89	0.54
1:B:31:HIS:CG	1:B:66:LEU:HD22	2.43	0.54
1:B:59:THR:O	1:B:62:GLU:N	2.40	0.54
1:C:148:ARG:CG	1:C:160:ALA:HB1	2.36	0.54
1:C:50:ILE:C	1:C:50:ILE:HD12	2.28	0.54
1:C:115:THR:HG22	1:C:116:ASN:N	2.21	0.54
1:C:120:MET:CE	1:C:132:ALA:HB3	2.37	0.54
1:E:65:LYS:HG3	1:E:66:LEU:N	2.17	0.54
1:A:14:ARG:HB2	1:A:18:TYR:CE1	2.41	0.54
1:B:5:GLU:HA	1:B:5:GLU:OE1	2.06	0.54
1:C:138:TRP:NE1	1:C:146:ALA:HB2	2.23	0.54
1:A:100:ILE:O	1:A:104:PHE:HB2	2.08	0.54
1:B:32:LEU:C	1:B:32:LEU:HD23	2.28	0.54
1:B:53:ASN:HD22	1:B:53:ASN:N	2.05	0.54
1:D:17:ILE:HG22	1:D:18:TYR:N	2.23	0.54
1:E:65:LYS:O	1:E:69:GLN:HG3	2.08	0.54
1:D:140:ALA:O	1:D:143:PRO:HG3	2.08	0.54
1:A:119:ARG:HG2	1:A:119:ARG:NH1	2.23	0.54
1:A:27:ILE:HD13	1:A:46:LEU:HD11	1.89	0.54
1:E:100:ILE:HA	1:E:103:VAL:HG12	1.88	0.54
1:E:16:LYS:HG3	1:E:57:VAL:HG22	1.89	0.54
1:B:120:MET:SD	1:B:129:ALA:HA	2.48	0.54
1:E:14:ARG:C	1:E:15:LEU:HD23	2.27	0.54
1:A:46:LEU:O	1:A:49:ALA:N	2.41	0.53
1:B:43:LYS:O	1:B:46:LEU:HB3	2.08	0.53
1:A:102:MET:O	1:A:106:MET:HG3	2.09	0.53
1:C:142:THR:N	1:C:143:PRO:HD3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:O	1:A:143:PRO:HD3	2.08	0.53
1:C:46:LEU:O	1:C:49:ALA:HB3	2.08	0.53
1:E:26:THR:HG21	1:E:30:GLY:HA2	1.90	0.53
1:C:81:ASN:HB3	1:C:84:LEU:HB2	1.91	0.53
1:A:79:LEU:CA	1:A:85:LYS:HG3	2.36	0.53
1:E:31:HIS:NE2	1:E:66:LEU:HD22	2.23	0.53
1:E:72:ASP:O	1:E:76:ARG:HG3	2.09	0.53
1:B:148:ARG:HB3	1:B:161:TYR:OH	2.09	0.53
1:A:16:LYS:HB2	1:A:57:VAL:CG2	2.30	0.52
1:D:148:ARG:HG2	1:D:160:ALA:O	2.09	0.52
1:B:68:ASN:O	1:B:72:ASP:OD1	2.27	0.52
1:C:69:GLN:O	1:C:72:ASP:HB2	2.08	0.52
1:E:26:THR:HG22	1:E:27:ILE:H	1.75	0.52
1:A:11:GLU:OE2	1:A:145:ARG:NH1	2.43	0.52
1:C:159:ASP:OD1	1:C:162:LYS:HE2	2.09	0.52
1:A:143:PRO:O	1:A:147:LYS:HG3	2.10	0.52
1:B:52:ARG:NH1	1:B:54:CYS:HA	2.25	0.52
1:E:50:ILE:HD11	1:E:54:CYS:SG	2.49	0.52
1:C:3:ILE:HG23	1:C:67:PHE:HE2	1.75	0.52
1:C:79:LEU:HA	1:C:85:LYS:HG3	1.91	0.52
1:A:24:TYR:CE1	1:E:96:ARG:NH1	2.77	0.52
1:A:1:MET:CG	1:A:2:ASN:H	2.23	0.51
1:C:97:CYS:SG	1:D:37:PRO:HG2	2.50	0.51
1:A:141:ALA:C	1:A:143:PRO:HD3	2.31	0.51
1:A:145:ARG:CA	1:A:148:ARG:NH2	2.72	0.51
1:D:84:LEU:CD1	1:D:108:GLU:HG2	2.40	0.51
1:C:162:LYS:HB3	1:C:162:LYS:HZ2	1.73	0.51
1:A:95:ARG:CG	1:A:95:ARG:HH11	2.24	0.51
1:C:14:ARG:HD2	1:C:18:TYR:CD1	2.44	0.51
1:B:114:PHE:HB3	1:B:117:SER:HB3	1.93	0.51
1:C:113:GLY:O	1:C:115:THR:N	2.35	0.51
1:D:13:LEU:HD11	1:D:15:LEU:CD2	2.41	0.51
1:D:33:LEU:C	1:D:34:THR:HG22	2.31	0.51
1:E:4:PHE:CD1	1:E:29:ILE:HD11	2.45	0.51
1:A:6:MET:O	1:A:10:ASP:OD1	2.29	0.51
1:A:7:LEU:HD12	1:A:67:PHE:CE1	2.46	0.51
1:B:137:ALA:O	1:B:140:ALA:HB3	2.11	0.51
1:C:46:LEU:HG	1:C:47:ASP:N	2.26	0.51
1:E:148:ARG:HG2	1:E:160:ALA:HB1	1.93	0.51
1:A:87:VAL:HG21	1:A:118:LEU:HB3	1.93	0.51
1:B:147:LYS:O	1:B:150:ILE:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:CG1	1:B:36:SER:HB2	2.41	0.51
1:D:87:VAL:HA	1:D:90:SER:OG	2.11	0.51
1:A:116:ASN:HD22	1:A:119:ARG:CD	2.23	0.51
1:C:26:THR:HG23	1:C:31:HIS:C	2.31	0.51
1:E:105:GLN:HG2	1:E:105:GLN:O	2.11	0.51
1:E:85:LYS:HB3	1:E:86:PRO:HD3	1.92	0.51
1:B:148:ARG:HD2	1:B:161:TYR:CZ	2.46	0.50
1:D:38:SER:HB3	1:D:41:ALA:CB	2.40	0.50
1:C:162:LYS:HB3	1:C:162:LYS:HZ3	1.74	0.50
1:C:15:LEU:O	1:C:57:VAL:HG13	2.12	0.50
1:D:8:ARG:NH2	1:D:9:ILE:CD1	2.71	0.50
1:B:1:MET:HE3	1:B:5:GLU:CG	2.39	0.50
1:C:13:LEU:HD12	1:C:29:ILE:HG13	1.93	0.50
1:E:114:PHE:HB3	1:E:117:SER:HB2	1.92	0.50
1:E:141:ALA:O	1:E:143:PRO:HD3	2.11	0.50
1:C:131:ALA:O	1:C:134:ALA:HB3	2.12	0.50
1:C:155:THR:OG1	1:C:157:THR:HG23	2.11	0.50
1:C:24:TYR:CE1	1:C:35:LYS:HB2	2.47	0.50
1:E:130:ALA:CB	1:E:154:ARG:HG3	2.42	0.50
1:B:10:ASP:OD1	1:B:148:ARG:NE	2.42	0.50
1:C:24:TYR:CE1	1:C:35:LYS:CB	2.95	0.50
1:D:78:ILE:HG23	1:D:84:LEU:HB3	1.94	0.50
1:E:64:GLU:O	1:E:67:PHE:HB3	2.12	0.50
1:D:20:ASP:OD1	1:D:22:GLU:N	2.38	0.50
1:A:40:ASN:OD1	1:E:68:ASN:OD1	2.29	0.50
1:A:36:SER:C	1:A:38:SER:H	2.15	0.50
1:A:46:LEU:O	1:A:49:ALA:HB3	2.12	0.50
1:B:115:THR:HG23	1:B:119:ARG:NH1	2.27	0.50
1:B:162:LYS:HB3	1:B:162:LYS:NZ	2.27	0.50
1:B:81:ASN:ND2	1:B:84:LEU:HD12	2.27	0.50
1:C:144:ASN:O	1:C:147:LYS:HB2	2.12	0.50
1:B:18:TYR:HD1	1:B:19:LYS:O	1.94	0.49
1:D:129:ALA:O	1:D:132:ALA:HB3	2.11	0.49
1:D:25:TYR:CE1	1:D:39:LEU:HD12	2.47	0.49
1:D:17:ILE:CG2	1:D:25:TYR:HD1	2.25	0.49
1:D:3:ILE:HG12	1:D:67:PHE:CZ	2.47	0.49
1:E:133:LEU:O	1:E:136:ALA:HB3	2.12	0.49
1:C:1:MET:HE3	1:C:5:GLU:HB3	1.95	0.49
1:C:72:ASP:HB3	1:C:76:ARG:HH22	1.75	0.49
1:D:17:ILE:O	1:D:18:TYR:HB3	2.12	0.49
1:B:7:LEU:HD23	1:B:11:GLU:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ALA:O	1:A:131:ALA:HB3	2.12	0.49
1:A:38:SER:HB3	1:A:41:ALA:HB2	1.95	0.49
1:B:32:LEU:HD23	1:B:34:THR:N	2.27	0.49
1:B:39:LEU:CD1	1:B:43:LYS:HD2	2.41	0.49
1:C:105:GLN:HB2	1:C:145:ARG:CZ	2.43	0.49
1:C:32:LEU:HG	1:C:33:LEU:N	2.24	0.49
1:D:146:ALA:O	1:D:150:ILE:HD12	2.12	0.49
1:A:4:PHE:CE1	1:A:64:GLU:HA	2.48	0.49
1:B:4:PHE:HD1	1:B:67:PHE:CD2	2.30	0.49
1:C:5:GLU:O	1:C:8:ARG:HB3	2.13	0.49
1:D:33:LEU:HD13	1:D:46:LEU:HB2	1.94	0.49
1:D:67:PHE:O	1:D:70:ASP:N	2.45	0.49
1:E:17:ILE:HD11	1:E:56:GLY:HA2	1.94	0.49
1:B:115:THR:O	1:B:119:ARG:HD2	2.12	0.49
1:A:106:MET:O	1:A:107:GLY:O	2.31	0.49
1:C:68:ASN:OD1	1:D:40:ASN:OD1	2.30	0.49
1:B:13:LEU:HG	1:B:14:ARG:N	2.28	0.49
1:D:50:ILE:HD13	1:D:62:GLU:CD	2.33	0.49
1:A:140:ALA:O	1:A:143:PRO:HG3	2.14	0.48
1:B:89:ASP:O	1:B:96:ARG:NH2	2.45	0.48
1:C:1:MET:HB3	1:C:158:TRP:CD1	2.48	0.48
1:A:20:ASP:OD1	1:A:22:GLU:N	2.46	0.48
1:C:103:VAL:HG23	1:C:111:VAL:HG21	1.95	0.48
1:C:105:GLN:OE1	1:C:145:ARG:HD3	2.13	0.48
1:A:103:VAL:HG22	1:A:111:VAL:HG21	1.95	0.48
1:A:14:ARG:HG3	1:A:18:TYR:CZ	2.47	0.48
1:D:131:ALA:O	1:D:134:ALA:HB3	2.13	0.48
1:D:120:MET:CE	1:D:129:ALA:HA	2.32	0.48
1:B:158:TRP:C	1:B:162:LYS:HG2	2.33	0.48
1:B:18:TYR:CZ	1:B:26:THR:HG22	2.49	0.48
1:D:28:GLY:O	1:D:30:GLY:N	2.42	0.48
1:A:59:THR:HG23	1:A:62:GLU:CG	2.43	0.48
1:B:106:MET:O	1:B:106:MET:HG3	2.13	0.48
1:B:118:LEU:O	1:B:121:LEU:HB2	2.13	0.48
1:C:148:ARG:HB3	1:C:161:TYR:CZ	2.49	0.48
1:C:140:ALA:O	1:C:143:PRO:HG3	2.13	0.48
1:C:130:ALA:HB1	1:C:150:ILE:CG2	2.44	0.48
1:D:34:THR:CG2	1:D:42:ALA:HA	2.42	0.48
1:A:93:ALA:O	1:A:96:ARG:HB2	2.13	0.48
1:B:34:THR:HG22	1:B:42:ALA:HB2	1.96	0.48
1:C:93:ALA:HA	1:C:96:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ARG:NH2	1:E:9:ILE:CG1	2.75	0.48
1:C:126:TRP:HA	1:C:126:TRP:HE3	1.78	0.47
1:B:162:LYS:NZ	1:B:162:LYS:CB	2.77	0.47
1:D:8:ARG:NH2	1:D:9:ILE:CG1	2.78	0.47
1:E:4:PHE:CA	1:E:67:PHE:CE2	2.96	0.47
1:A:133:LEU:C	1:A:135:ALA:H	2.17	0.47
1:B:105:GLN:CG	1:B:145:ARG:NH1	2.78	0.47
1:C:39:LEU:HD12	1:C:39:LEU:O	2.15	0.47
1:D:142:THR:N	1:D:143:PRO:CD	2.78	0.47
1:D:15:LEU:HD13	1:D:58:ILE:O	2.13	0.47
1:A:51:GLY:O	1:A:52:ARG:HB3	2.14	0.47
1:A:3:ILE:HB	1:A:97:CYS:SG	2.54	0.47
1:B:129:ALA:O	1:B:133:LEU:HD12	2.14	0.47
1:B:131:ALA:O	1:B:134:ALA:HB3	2.15	0.47
1:B:60:LYS:HB3	1:B:60:LYS:HE3	1.47	0.47
1:A:75:VAL:HA	1:A:78:ILE:HD12	1.96	0.47
1:B:59:THR:HG23	1:B:62:GLU:OE2	2.14	0.47
1:C:7:LEU:HD22	1:C:11:GLU:CG	2.45	0.47
1:D:138:TRP:HH2	1:D:149:VAL:HG12	1.80	0.47
1:D:18:TYR:O	1:D:26:THR:N	2.41	0.47
1:D:27:ILE:CD1	1:D:58:ILE:HG12	2.45	0.47
1:E:8:ARG:HG2	1:E:8:ARG:O	2.13	0.47
1:C:114:PHE:HB3	1:C:117:SER:CB	2.44	0.47
1:D:17:ILE:CG2	1:D:18:TYR:N	2.76	0.47
1:A:131:ALA:O	1:A:133:LEU:N	2.48	0.47
1:A:33:LEU:C	1:A:34:THR:HG22	2.35	0.47
1:C:155:THR:OG1	1:C:157:THR:N	2.48	0.47
1:C:87:VAL:HG12	1:C:87:VAL:O	2.14	0.47
1:C:87:VAL:O	1:C:91:LEU:HG	2.15	0.47
1:D:140:ALA:O	1:D:143:PRO:HD3	2.14	0.47
1:A:7:LEU:CD1	1:A:67:PHE:HE1	2.27	0.47
1:B:1:MET:HB3	1:B:158:TRP:CD1	2.50	0.47
1:E:120:MET:HE1	1:E:132:ALA:HB2	1.97	0.47
1:D:93:ALA:CB	1:E:19:LYS:HZ1	2.28	0.47
1:A:148:ARG:HG2	1:A:160:ALA:HB1	1.97	0.47
1:A:29:ILE:O	1:A:29:ILE:HG22	2.14	0.47
1:D:8:ARG:O	1:D:12:GLY:HA2	2.15	0.47
1:A:45:GLU:OE1	1:A:48:LYS:HE2	2.14	0.46
1:E:162:LYS:NZ	1:E:162:LYS:CB	2.78	0.46
1:A:34:THR:HG21	1:A:42:ALA:HA	1.97	0.46
1:B:117:SER:HA	1:B:120:MET:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:CG2	1:A:42:ALA:HA	2.45	0.46
1:B:105:GLN:CB	1:B:145:ARG:NH1	2.78	0.46
1:D:1:MET:HG3	1:D:2:ASN:H	1.79	0.46
1:D:93:ALA:HB2	1:E:19:LYS:HZ3	1.80	0.46
1:A:95:ARG:CD	1:A:126:TRP:CH2	2.99	0.46
1:A:26:THR:CG2	1:A:27:ILE:N	2.79	0.46
1:A:50:ILE:HG22	1:A:66:LEU:HD21	1.97	0.46
1:E:4:PHE:HB2	1:E:67:PHE:CE2	2.51	0.46
1:B:1:MET:HB3	1:B:158:TRP:CE2	2.48	0.46
1:D:111:VAL:O	1:D:118:LEU:HD11	2.16	0.46
1:D:124:LYS:HA	1:D:126:TRP:CH2	2.50	0.46
1:E:50:ILE:HD11	1:E:52:ARG:HE	1.80	0.46
1:A:94:VAL:CG2	1:A:158:TRP:CE2	2.99	0.46
1:B:105:GLN:NE2	1:B:145:ARG:CD	2.79	0.46
1:E:6:MET:HE1	1:E:101:ASN:HB3	1.98	0.46
1:B:50:ILE:CG1	1:B:51:GLY:N	2.74	0.46
1:B:87:VAL:HG22	1:B:122:GLN:HE21	1.81	0.46
1:E:26:THR:CG2	1:E:27:ILE:N	2.77	0.46
1:E:58:ILE:HG22	1:E:62:GLU:OE1	2.16	0.46
1:B:85:LYS:HE3	1:B:89:ASP:OD2	2.16	0.46
1:E:3:ILE:HG23	1:E:67:PHE:HE2	1.80	0.46
1:A:133:LEU:O	1:A:135:ALA:N	2.50	0.45
1:A:95:ARG:CG	1:A:95:ARG:NH1	2.79	0.45
1:D:9:ILE:HG21	1:D:161:TYR:HD2	1.81	0.45
1:A:115:THR:HG22	1:A:116:ASN:HD22	1.81	0.45
1:D:115:THR:O	1:D:119:ARG:HD2	2.17	0.45
1:C:143:PRO:O	1:C:147:LYS:HD2	2.16	0.45
1:C:145:ARG:C	1:C:147:LYS:H	2.18	0.45
1:A:18:TYR:CE1	1:A:26:THR:HG22	2.52	0.45
1:C:87:VAL:HG21	1:C:118:LEU:HB3	1.97	0.45
1:A:105:GLN:HB2	1:A:145:ARG:CZ	2.47	0.45
1:A:32:LEU:C	1:A:32:LEU:HD23	2.36	0.45
1:A:85:LYS:N	1:A:86:PRO:CD	2.79	0.45
1:B:105:GLN:HE21	1:B:145:ARG:NH1	2.09	0.45
1:C:119:ARG:O	1:C:123:GLN:HG2	2.17	0.45
1:A:87:VAL:HA	1:A:122:GLN:CG	2.47	0.45
1:A:159:ASP:CA	1:A:162:LYS:HE2	2.46	0.45
1:B:18:TYR:CZ	1:B:26:THR:CG2	3.00	0.45
1:C:102:MET:CE	1:C:111:VAL:HG13	2.44	0.45
1:D:143:PRO:O	1:D:147:LYS:HG3	2.17	0.45
1:C:96:ARG:O	1:C:100:ILE:HD12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HG23	1:B:84:LEU:HB3	1.98	0.45
1:C:14:ARG:HD2	1:C:18:TYR:CG	2.51	0.45
1:C:3:ILE:HG12	1:C:67:PHE:CZ	2.43	0.45
1:E:120:MET:CE	1:E:132:ALA:HB2	2.47	0.45
1:A:88:TYR:CE1	1:A:96:ARG:HD3	2.52	0.45
1:B:70:ASP:O	1:B:73:ALA:HB3	2.17	0.45
1:C:7:LEU:CD2	1:C:11:GLU:HG2	2.47	0.45
1:C:72:ASP:O	1:C:76:ARG:HB2	2.16	0.45
1:A:117:SER:OG	1:A:133:LEU:HD21	2.18	0.44
1:B:1:MET:CB	1:B:158:TRP:CG	2.97	0.44
1:B:6:MET:CE	1:B:158:TRP:CZ3	3.00	0.44
1:C:120:MET:HE1	1:C:132:ALA:HB3	1.98	0.44
1:D:105:GLN:HB2	1:D:145:ARG:NH2	2.32	0.44
1:D:20:ASP:OD2	1:D:24:TYR:HB2	2.16	0.44
1:D:94:VAL:O	1:D:97:CYS:HB2	2.18	0.44
1:E:33:LEU:HA	1:E:33:LEU:HD23	1.44	0.44
1:D:79:LEU:CD1	1:E:35:LYS:HD2	2.47	0.44
1:C:120:MET:HE2	1:C:132:ALA:HB3	1.98	0.44
1:C:24:TYR:CD1	1:C:35:LYS:CB	2.98	0.44
1:D:71:VAL:O	1:D:74:ALA:HB3	2.18	0.44
1:D:88:TYR:CZ	1:D:96:ARG:HD3	2.52	0.44
1:A:79:LEU:HD21	1:A:88:TYR:CD2	2.52	0.44
1:E:81:ASN:OD1	1:E:82:ALA:N	2.50	0.44
1:A:95:ARG:CD	1:A:126:TRP:CZ3	3.01	0.44
1:A:142:THR:N	1:A:143:PRO:HD3	2.33	0.44
1:A:81:ASN:HD22	1:A:84:LEU:HD12	1.78	0.44
1:B:103:VAL:O	1:B:107:GLY:N	2.51	0.44
1:E:8:ARG:NH2	1:E:9:ILE:CD1	2.80	0.44
1:A:103:VAL:HA	1:A:111:VAL:HG21	1.99	0.44
1:A:119:ARG:HH11	1:A:119:ARG:CG	2.29	0.44
1:C:6:MET:SD	1:C:158:TRP:HZ3	2.41	0.44
1:A:15:LEU:O	1:A:57:VAL:HG13	2.17	0.44
1:A:2:ASN:OD1	1:A:2:ASN:N	2.49	0.44
1:A:47:ASP:HA	1:A:54:CYS:SG	2.57	0.44
1:B:1:MET:HE3	1:B:5:GLU:CB	2.46	0.44
1:C:50:ILE:HD11	1:C:54:CYS:SG	2.57	0.44
1:A:114:PHE:HB3	1:A:117:SER:HB3	1.99	0.44
1:A:119:ARG:NH1	1:A:119:ARG:CG	2.81	0.44
1:D:13:LEU:HD11	1:D:15:LEU:HD21	2.00	0.44
1:A:38:SER:HB3	1:A:41:ALA:CB	2.48	0.44
1:B:3:ILE:HD13	1:B:71:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:TRP:HA	1:C:126:TRP:CE3	2.51	0.44
1:C:18:TYR:O	1:C:25:TYR:HA	2.17	0.44
1:D:143:PRO:O	1:D:147:LYS:HD2	2.18	0.44
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.76	0.43
1:B:114:PHE:HB3	1:B:117:SER:CB	2.48	0.43
1:D:25:TYR:HE1	1:D:39:LEU:HD12	1.83	0.43
1:D:72:ASP:O	1:D:76:ARG:HB2	2.19	0.43
1:B:14:ARG:HB2	1:B:18:TYR:CE2	2.52	0.43
1:C:120:MET:HE2	1:C:132:ALA:CB	2.48	0.43
1:B:25:TYR:CE2	1:B:38:SER:O	2.71	0.43
1:C:60:LYS:NZ	1:C:60:LYS:O	2.40	0.43
1:E:8:ARG:O	1:E:12:GLY:HA2	2.17	0.43
1:E:1:MET:HE2	1:E:5:GLU:C	2.38	0.43
1:B:117:SER:OG	1:B:133:LEU:HG	2.19	0.43
1:C:46:LEU:O	1:C:49:ALA:N	2.51	0.43
1:D:52:ARG:O	1:D:54:CYS:N	2.46	0.43
1:A:115:THR:CG2	1:A:119:ARG:HD2	2.45	0.43
1:D:39:LEU:HD21	1:D:43:LYS:HZ1	1.84	0.43
1:A:155:THR:OG1	1:A:157:THR:OG1	2.27	0.43
1:C:10:ASP:OD1	1:C:161:TYR:HE2	2.02	0.43
1:E:116:ASN:N	1:E:116:ASN:ND2	2.64	0.43
1:E:67:PHE:O	1:E:70:ASP:HB2	2.19	0.43
1:B:46:LEU:HD11	1:B:50:ILE:CG2	2.49	0.43
1:B:58:ILE:HB	1:B:62:GLU:OE1	2.19	0.43
1:C:14:ARG:C	1:C:15:LEU:HG	2.39	0.43
1:D:10:ASP:CB	1:D:145:ARG:HG3	2.49	0.43
1:E:14:ARG:HB2	1:E:18:TYR:CE1	2.54	0.43
1:A:96:ARG:HB2	1:B:37:PRO:HG3	2.00	0.43
1:C:120:MET:HE3	1:C:129:ALA:HA	1.93	0.42
1:C:29:ILE:O	1:C:29:ILE:HG22	2.19	0.42
1:D:29:ILE:HG22	1:D:29:ILE:O	2.19	0.42
1:E:10:ASP:OD1	1:E:161:TYR:HE1	2.01	0.42
1:E:8:ARG:NH2	1:E:9:ILE:HD11	2.34	0.42
1:B:4:PHE:HA	1:B:67:PHE:CE2	2.55	0.42
1:E:118:LEU:O	1:E:122:GLN:HB2	2.19	0.42
1:E:17:ILE:HG13	1:E:56:GLY:CA	2.50	0.42
1:A:94:VAL:CG2	1:A:158:TRP:NE1	2.82	0.42
1:A:24:TYR:CE1	1:A:35:LYS:CB	2.98	0.42
1:A:71:VAL:CG1	1:B:36:SER:CB	2.98	0.42
1:D:148:ARG:HB3	1:D:161:TYR:CZ	2.54	0.42
1:E:36:SER:HA	1:E:37:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ALA:O	1:B:45:GLU:N	2.42	0.42
1:D:15:LEU:O	1:D:57:VAL:HA	2.19	0.42
1:E:10:ASP:OD2	1:E:101:ASN:ND2	2.50	0.42
1:A:65:LYS:HG3	1:A:66:LEU:N	2.28	0.42
1:A:88:TYR:CD1	1:A:96:ARG:HD3	2.54	0.42
1:C:34:THR:CG2	1:C:42:ALA:HA	2.49	0.42
1:E:145:ARG:HH11	1:E:145:ARG:HD2	1.71	0.42
1:A:150:ILE:HG22	1:A:150:ILE:O	2.20	0.42
1:A:7:LEU:HD12	1:A:67:PHE:CZ	2.55	0.42
1:B:134:ALA:C	1:B:136:ALA:H	2.23	0.42
1:C:6:MET:CE	1:C:101:ASN:ND2	2.83	0.42
1:C:7:LEU:HA	1:C:7:LEU:HD23	1.89	0.42
1:E:88:TYR:CZ	1:E:96:ARG:HD3	2.55	0.42
1:A:36:SER:HB2	1:E:71:VAL:HG12	2.02	0.42
1:B:148:ARG:HD2	1:B:161:TYR:CD2	2.54	0.42
1:B:62:GLU:O	1:B:65:LYS:HB3	2.19	0.42
1:D:6:MET:SD	1:D:101:ASN:ND2	2.87	0.42
1:B:92:ASP:O	1:B:96:ARG:HG2	2.20	0.42
1:D:91:LEU:HD13	1:D:95:ARG:HB3	2.02	0.42
1:D:8:ARG:NE	1:D:9:ILE:HG13	2.35	0.42
1:A:131:ALA:O	1:A:134:ALA:N	2.53	0.42
1:B:26:THR:CG2	1:B:27:ILE:N	2.83	0.42
1:C:120:MET:CE	1:C:132:ALA:CB	2.97	0.42
1:C:1:MET:HE3	1:C:5:GLU:CB	2.49	0.42
1:B:60:LYS:O	1:B:60:LYS:NZ	2.53	0.41
1:A:94:VAL:O	1:A:97:CYS:HB2	2.20	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.72	0.41
1:C:103:VAL:HA	1:C:111:VAL:HG21	2.02	0.41
1:C:98:ALA:HB3	1:C:153:PHE:CE1	2.54	0.41
1:D:36:SER:HA	1:D:37:PRO:HD3	1.90	0.41
1:D:3:ILE:HG23	1:D:67:PHE:HE2	1.85	0.41
1:B:31:HIS:HD2	1:B:33:LEU:CD2	2.33	0.41
1:C:99:LEU:HA	1:C:99:LEU:HD12	1.75	0.41
1:D:120:MET:HE3	1:D:132:ALA:CB	2.51	0.41
1:C:71:VAL:CG1	1:D:36:SER:HB2	2.50	0.41
1:E:108:GLU:O	1:E:110:GLY:N	2.53	0.41
1:A:44:SER:O	1:A:48:LYS:HB2	2.21	0.41
1:B:58:ILE:HB	1:B:59:THR:H	1.57	0.41
1:D:32:LEU:HD23	1:D:33:LEU:N	2.36	0.41
1:D:94:VAL:HG22	1:D:158:TRP:CE2	2.55	0.41
1:E:79:LEU:O	1:E:85:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:HIS:CD2	1:B:33:LEU:HD23	2.55	0.41
1:C:111:VAL:C	1:C:113:GLY:H	2.24	0.41
1:C:50:ILE:HG12	1:C:54:CYS:SG	2.60	0.41
1:D:60:LYS:HZ2	1:D:60:LYS:C	2.18	0.41
1:E:6:MET:HE1	1:E:101:ASN:CB	2.51	0.41
1:E:88:TYR:CE1	1:E:96:ARG:HB3	2.55	0.41
1:B:77:GLY:O	1:B:80:ARG:N	2.54	0.41
1:C:148:ARG:O	1:C:152:THR:OG1	2.34	0.41
1:C:15:LEU:HB3	1:C:58:ILE:CG1	2.50	0.41
1:A:10:ASP:OD1	1:A:161:TYR:HE2	2.03	0.41
1:C:26:THR:CG2	1:C:27:ILE:N	2.83	0.41
1:C:92:ASP:OD1	1:C:95:ARG:HG3	2.20	0.41
1:D:18:TYR:HD1	1:D:19:LYS:O	2.04	0.41
1:E:85:LYS:HB3	1:E:86:PRO:CD	2.51	0.41
1:B:115:THR:HG23	1:B:119:ARG:HH11	1.84	0.41
1:B:14:ARG:HB2	1:B:18:TYR:HE2	1.85	0.41
1:C:3:ILE:HG23	1:C:67:PHE:CE2	2.54	0.41
1:A:3:ILE:HD12	1:A:100:ILE:HD13	2.03	0.41
1:A:75:VAL:O	1:A:78:ILE:N	2.54	0.41
1:B:52:ARG:O	1:B:54:CYS:N	2.54	0.41
1:E:111:VAL:O	1:E:113:GLY:N	2.53	0.41
1:A:3:ILE:CD1	1:A:71:VAL:CG2	2.99	0.40
1:B:115:THR:O	1:B:119:ARG:HG3	2.22	0.40
1:B:14:ARG:O	1:B:28:GLY:HA2	2.20	0.40
1:C:75:VAL:HG12	1:C:79:LEU:CD1	2.51	0.40
1:D:14:ARG:HG3	1:D:18:TYR:CD2	2.53	0.40
1:E:85:LYS:N	1:E:86:PRO:HD2	2.35	0.40
1:A:16:LYS:HA	1:A:56:GLY:O	2.21	0.40
1:A:1:MET:HG3	1:A:2:ASN:H	1.86	0.40
1:B:46:LEU:HD12	1:B:50:ILE:HG23	2.02	0.40
1:B:60:LYS:HZ2	1:B:60:LYS:C	2.24	0.40
1:C:9:ILE:HG22	1:C:10:ASP:N	2.36	0.40
1:D:39:LEU:HD21	1:D:43:LYS:NZ	2.36	0.40
1:A:1:MET:HG3	1:A:5:GLU:HB2	2.04	0.40
1:A:114:PHE:O	1:A:117:SER:HB3	2.21	0.40
1:A:88:TYR:CE1	1:A:96:ARG:CD	3.05	0.40
1:D:155:THR:OG1	1:D:157:THR:OG1	2.27	0.40
1:D:3:ILE:O	1:D:6:MET:HB3	2.22	0.40
1:E:17:ILE:HG13	1:E:56:GLY:HA3	2.04	0.40
1:A:7:LEU:CD1	1:A:67:PHE:CE1	3.05	0.40
1:B:114:PHE:O	1:B:117:SER:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD22	1:C:35:LYS:CD	2.52	0.40
1:C:75:VAL:CG1	1:C:79:LEU:CD1	2.99	0.40
1:D:1:MET:CB	1:D:158:TRP:CG	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/164 (98%)	124 (78%)	22 (14%)	14 (9%)	1	3
1	B	160/164 (98%)	127 (79%)	26 (16%)	7 (4%)	2	15
1	C	160/164 (98%)	128 (80%)	28 (18%)	4 (2%)	5	28
1	D	160/164 (98%)	133 (83%)	19 (12%)	8 (5%)	2	12
1	E	160/164 (98%)	130 (81%)	21 (13%)	9 (6%)	2	10
All	All	800/820 (98%)	642 (80%)	116 (14%)	42 (5%)	2	11

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	93	ALA
1	A	115	THR
1	B	52	ARG
1	B	126	TRP
1	B	160	ALA
1	C	114	PHE
1	D	29	ILE
1	D	143	PRO
1	E	3	ILE
1	A	107	GLY

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Mol	Chain	Res	Type
1	A	126	TRP
1	A	132	ALA
1	B	115	THR
1	B	135	ALA
1	C	107	GLY
1	C	115	THR
1	E	70	ASP
1	E	107	GLY
1	E	108	GLU
1	E	109	THR
1	E	115	THR
1	E	136	ALA
1	A	37	PRO
1	A	46	LEU
1	A	131	ALA
1	A	134	ALA
1	B	53	ASN
1	D	137	ALA
1	A	155	THR
1	D	53	ASN
1	D	55	ASN
1	D	60	LYS
1	D	160	ALA
1	E	131	ALA
1	A	137	ALA
1	A	154	ARG
1	D	142	THR
1	A	17	ILE
1	C	85	LYS
1	E	17	ILE
1	B	29	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	127/129 (98%)	97 (76%)	30 (24%)	1	3
1	B	127/129 (98%)	99 (78%)	28 (22%)	1	4
1	C	127/129 (98%)	92 (72%)	35 (28%)	0	2
1	D	127/129 (98%)	101 (80%)	26 (20%)	1	6
1	E	127/129 (98%)	96 (76%)	31 (24%)	0	3
All	All	635/645 (98%)	485 (76%)	150 (24%)	1	3

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	ASP
1	A	13	LEU
1	A	17	ILE
1	A	34	THR
1	A	35	LYS
1	A	36	SER
1	A	43	LYS
1	A	44	SER
1	A	48	LYS
1	A	50	ILE
1	A	53	ASN
1	A	54	CYS
1	A	58	ILE
1	A	59	THR
1	A	60	LYS
1	A	80	ARG
1	A	85	LYS
1	A	95	ARG
1	A	99	LEU
1	A	103	VAL
1	A	104	PHE
1	A	106	MET
1	A	119	ARG
1	A	122	GLN
1	A	145	ARG
1	A	151	THR
1	A	154	ARG

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Mol	Chain	Res	Type
1	A	155	THR
1	A	162	LYS
1	B	1	MET
1	B	5	GLU
1	B	13	LEU
1	B	16	LYS
1	B	29	ILE
1	B	38	SER
1	B	43	LYS
1	B	45	GLU
1	B	50	ILE
1	B	53	ASN
1	B	59	THR
1	B	60	LYS
1	B	79	LEU
1	B	83	LYS
1	B	85	LYS
1	B	90	SER
1	B	92	ASP
1	B	96	ARG
1	B	104	PHE
1	B	106	MET
1	B	117	SER
1	B	119	ARG
1	B	125	ARG
1	B	142	THR
1	B	147	LYS
1	B	150	ILE
1	B	154	ARG
1	B	162	LYS
1	C	1	MET
1	C	8	ARG
1	C	13	LEU
1	C	15	LEU
1	C	16	LYS
1	C	17	ILE
1	C	32	LEU
1	C	34	THR
1	C	36	SER
1	C	43	LYS
1	C	44	SER
1	C	53	ASN

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Mol	Chain	Res	Type
1	C	54	CYS
1	C	60	LYS
1	C	65	LYS
1	C	85	LYS
1	C	90	SER
1	C	96	ARG
1	C	102	MET
1	C	103	VAL
1	C	104	PHE
1	C	109	THR
1	C	116	ASN
1	C	119	ARG
1	C	123	GLN
1	C	124	LYS
1	C	125	ARG
1	C	126	TRP
1	C	127	ASP
1	C	148	ARG
1	C	150	ILE
1	C	152	THR
1	C	155	THR
1	C	157	THR
1	C	162	LYS
1	D	1	MET
1	D	6	MET
1	D	7	LEU
1	D	13	LEU
1	D	16	LYS
1	D	34	THR
1	D	39	LEU
1	D	43	LYS
1	D	48	LYS
1	D	50	ILE
1	D	52	ARG
1	D	53	ASN
1	D	59	THR
1	D	60	LYS
1	D	65	LYS
1	D	83	LYS
1	D	90	SER
1	D	104	PHE
1	D	106	MET

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Mol	Chain	Res	Type
1	D	109	THR
1	D	119	ARG
1	D	142	THR
1	D	145	ARG
1	D	149	VAL
1	D	155	THR
1	D	162	LYS
1	E	1	MET
1	E	8	ARG
1	E	14	ARG
1	E	15	LEU
1	E	16	LYS
1	E	35	LYS
1	E	36	SER
1	E	43	LYS
1	E	48	LYS
1	E	50	ILE
1	E	52	ARG
1	E	53	ASN
1	E	60	LYS
1	E	65	LYS
1	E	69	GLN
1	E	78	ILE
1	E	89	ASP
1	E	90	SER
1	E	92	ASP
1	E	97	CYS
1	E	99	LEU
1	E	104	PHE
1	E	115	THR
1	E	116	ASN
1	E	117	SER
1	E	119	ARG
1	E	124	LYS
1	E	125	ARG
1	E	145	ARG
1	E	154	ARG
1	E	162	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	116	ASN
1	B	31	HIS
1	B	40	ASN
1	B	53	ASN
1	B	105	GLN
1	B	116	ASN
1	B	122	GLN
1	B	144	ASN
1	C	31	HIS
1	C	53	ASN
1	C	69	GLN
1	C	101	ASN
1	C	116	ASN
1	C	122	GLN
1	D	40	ASN
1	D	53	ASN
1	D	68	ASN
1	D	116	ASN
1	D	122	GLN
1	E	31	HIS
1	E	53	ASN
1	E	116	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	162/164 (98%)	-0.67	0 100 100	4, 27, 48, 64	0
1	B	162/164 (98%)	-0.54	0 100 100	5, 29, 49, 64	0
1	C	162/164 (98%)	-0.68	0 100 100	4, 23, 55, 75	0
1	D	162/164 (98%)	-0.73	0 100 100	2, 22, 46, 63	0
1	E	162/164 (98%)	-0.72	0 100 100	5, 21, 45, 60	0
All	All	810/820 (98%)	-0.67	0 100 100	2, 24, 49, 75	0

There are no RSRZ outliers to report.

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 carbohydrates 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.