Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 06:17 PM GMT

PDB ID	:	168L
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	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

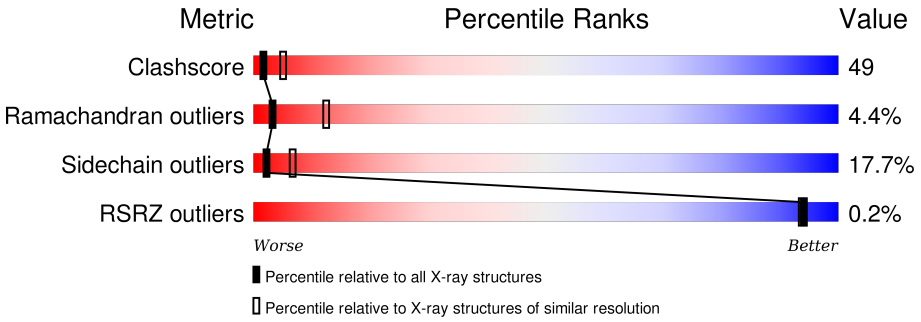
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	164	% 20% 57% 21%
1	B	164	34% 49% 16%
1	C	164	36% 47% 16%
1	D	164	34% 48% 16%
1	E	164	37% 47% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6445 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	164	Total	C	N	O	S	38	0	0
			1289	812	233	237	7			
1	B	164	Total	C	N	O	S	38	0	0
			1289	812	233	237	7			
1	C	164	Total	C	N	O	S	38	0	0
			1289	812	233	237	7			
1	D	164	Total	C	N	O	S	38	0	0
			1289	812	233	237	7			
1	E	164	Total	C	N	O	S	38	0	0
			1289	812	233	237	7			

There are 30 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
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
C	128	ALA	GLU	CONFLICT	UNP P00720
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
D	128	ALA	GLU	CONFLICT	UNP P00720

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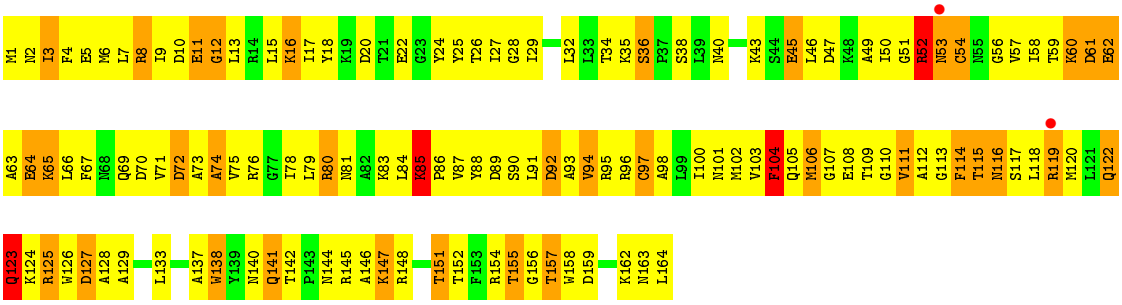
Chain	Residue	Modelled	Actual	Comment	Reference
D	131	ALA	VAL	CONFLICT	UNP P00720
D	132	ALA	ASN	CONFLICT	UNP P00720
D	135	ALA	LYS	CONFLICT	UNP P00720
D	136	ALA	SER	CONFLICT	UNP P00720
D	137	ALA	ARG	CONFLICT	UNP P00720
E	128	ALA	GLU	CONFLICT	UNP P00720
E	131	ALA	VAL	CONFLICT	UNP P00720
E	132	ALA	ASN	CONFLICT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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:

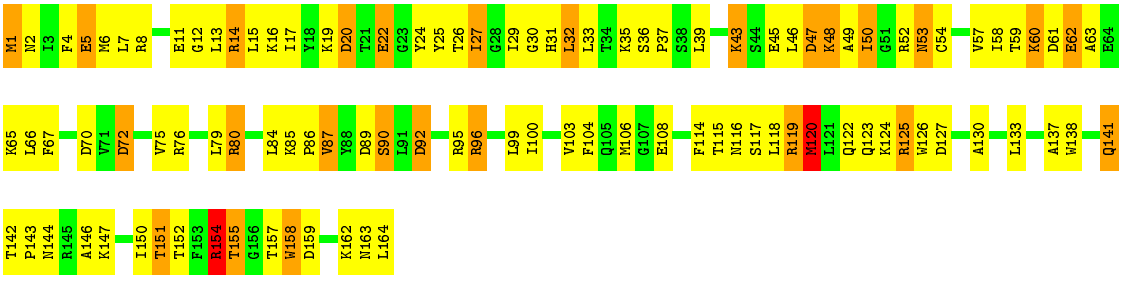


- Molecule 1: T4 LYSOZYME

Chain B:

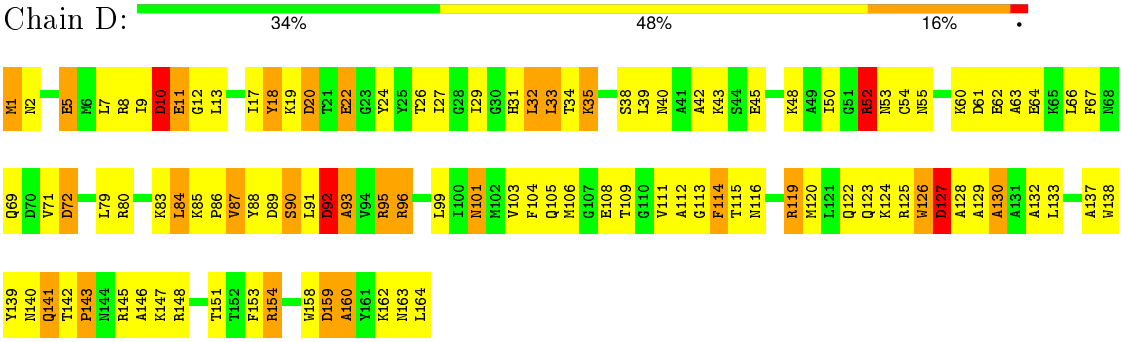
- Molecule 1: T4 LYSOZYME

Chain C:



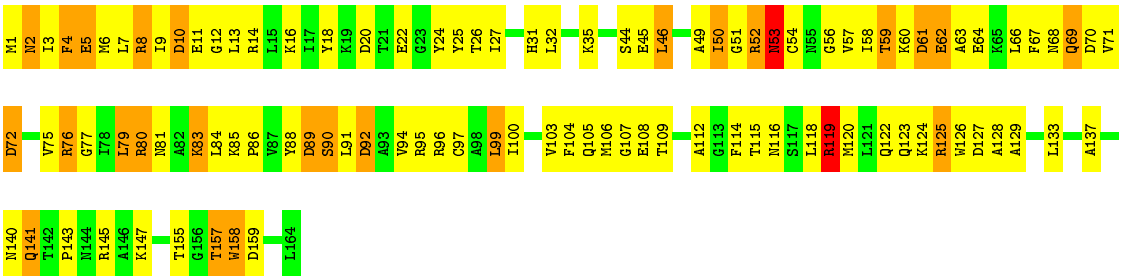
• Molecule 1: T4 LYSOZYME

Chain D:



• Molecule 1: T4 LYSOZYME

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	157.20Å 177.90Å 40.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90 11.83 – 2.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.90) 79.5 (11.83-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.83Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.199 , (Not available) 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 119.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 22098 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6445	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.02	5/1309 (0.4%)	1.54	19/1764 (1.1%)
1	B	1.12	6/1309 (0.5%)	1.62	26/1764 (1.5%)
1	C	1.14	6/1309 (0.5%)	1.63	25/1764 (1.4%)
1	D	1.04	6/1309 (0.5%)	1.53	16/1764 (0.9%)
1	E	1.04	8/1309 (0.6%)	2.13	30/1764 (1.7%)
All	All	1.07	31/6545 (0.5%)	1.70	116/8820 (1.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	22	GLU	CD-OE2	8.22	1.34	1.25
1	C	62	GLU	CD-OE2	7.97	1.34	1.25
1	E	22	GLU	CD-OE2	7.63	1.34	1.25
1	C	108	GLU	CD-OE1	7.58	1.33	1.25
1	D	22	GLU	CD-OE1	7.53	1.33	1.25
1	A	62	GLU	CD-OE2	7.32	1.33	1.25
1	E	5	GLU	CD-OE2	7.21	1.33	1.25
1	B	108	GLU	CD-OE2	7.03	1.33	1.25
1	E	89	ASP	CB-CG	-6.70	1.37	1.51
1	D	45	GLU	CD-OE1	6.62	1.32	1.25
1	D	108	GLU	CD-OE1	6.57	1.32	1.25
1	B	62	GLU	CD-OE2	6.46	1.32	1.25
1	E	108	GLU	CD-OE2	6.39	1.32	1.25
1	D	11	GLU	CD-OE2	6.28	1.32	1.25
1	C	11	GLU	CD-OE2	6.25	1.32	1.25
1	B	5	GLU	CD-OE2	6.21	1.32	1.25
1	E	64	GLU	CD-OE2	6.17	1.32	1.25
1	D	5	GLU	CD-OE2	6.12	1.32	1.25
1	C	22	GLU	CD-OE2	5.93	1.32	1.25
1	B	45	GLU	CD-OE2	5.92	1.32	1.25
1	A	64	GLU	CD-OE2	5.74	1.31	1.25
1	A	45	GLU	CD-OE2	5.73	1.31	1.25
1	C	45	GLU	CD-OE2	5.54	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	GLU	CD-OE2	5.51	1.31	1.25
1	C	5	GLU	CD-OE2	5.50	1.31	1.25
1	E	45	GLU	CD-OE2	5.46	1.31	1.25
1	E	11	GLU	CD-OE2	5.41	1.31	1.25
1	A	22	GLU	CD-OE1	5.40	1.31	1.25
1	B	64	GLU	CD-OE2	5.22	1.31	1.25
1	E	62	GLU	CD-OE2	5.21	1.31	1.25
1	D	64	GLU	CD-OE2	5.04	1.31	1.25

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	89	ASP	CB-CG-OD2	-40.53	81.82	118.30
1	E	89	ASP	CB-CG-OD1	40.12	154.41	118.30
1	E	70	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	D	10	ASP	CB-CG-OD1	-9.03	110.17	118.30
1	A	25	TYR	CB-CG-CD1	-8.51	115.89	121.00
1	B	70	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	B	61	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	E	70	ASP	CB-CG-OD1	8.18	125.66	118.30
1	C	72	ASP	CB-CG-OD2	-8.14	110.98	118.30
1	C	119	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	D	127	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	E	92	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	D	92	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	C	61	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	B	18	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	A	61	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	A	92	ASP	CB-CG-OD1	-7.66	111.40	118.30
1	E	89	ASP	O-C-N	-7.57	110.59	122.70
1	E	20	ASP	CB-CG-OD1	7.46	125.02	118.30
1	C	127	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	92	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	E	20	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	47	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	C	20	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	C	72	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	120	MET	CA-CB-CG	-7.26	100.96	113.30
1	A	72	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	E	61	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	11	GLU	CB-CA-C	-7.21	95.97	110.40
1	C	125	ARG	NE-CZ-NH1	7.14	123.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	70	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	61	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	D	20	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	B	80	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	C	20	ASP	CB-CG-OD1	7.03	124.62	118.30
1	C	47	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	127	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	89	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	E	159	ASP	CB-CG-OD1	6.79	124.41	118.30
1	D	20	ASP	CB-CG-OD1	6.72	124.35	118.30
1	E	159	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	E	79	LEU	CB-CA-C	6.65	122.83	110.20
1	E	10	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	E	127	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	127	ASP	CB-CG-OD1	-6.58	112.37	118.30
1	E	127	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	61	ASP	CB-CG-OD1	6.45	124.10	118.30
1	D	96	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	E	61	ASP	CB-CG-OD1	6.31	123.98	118.30
1	C	89	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	159	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	D	10	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	20	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	89	ASP	CB-CG-OD1	6.18	123.86	118.30
1	E	119	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	159	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	159	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	47	ASP	CB-CG-OD1	6.05	123.75	118.30
1	D	33	LEU	CB-CA-C	-6.03	98.74	110.20
1	B	89	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	52	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	72	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	E	92	ASP	CB-CG-OD1	5.93	123.64	118.30
1	E	8	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	74	ALA	N-CA-CB	-5.87	101.89	110.10
1	B	154	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	127	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	88	TYR	CB-CG-CD1	-5.84	117.49	121.00
1	D	80	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	125	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	B	61	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	72	ASP	CB-CG-OD2	-5.73	113.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	72	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	104	PHE	CB-CG-CD1	5.69	124.78	120.80
1	D	96	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	89	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	92	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	E	70	ASP	CA-C-N	-5.67	104.74	117.20
1	B	76	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	14	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	127	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	88	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	A	80	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	E	69	GLN	N-CA-CB	5.52	120.53	110.60
1	E	89	ASP	C-N-CA	5.51	135.47	121.70
1	B	145	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	B	120	MET	CA-CB-CG	-5.44	104.04	113.30
1	B	72	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	97	CYS	CA-CB-SG	-5.42	104.25	114.00
1	C	159	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	72	ASP	N-CA-CB	5.38	120.29	110.60
1	C	127	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	142	THR	C-N-CD	-5.33	108.88	120.60
1	C	154	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	48	LYS	CB-CA-C	-5.31	99.78	110.40
1	C	47	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	17	ILE	CB-CA-C	-5.30	101.00	111.60
1	E	89	ASP	CA-C-N	5.27	128.80	117.20
1	B	68	ASN	CB-CA-C	5.26	120.91	110.40
1	A	72	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	80	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	89	ASP	CB-CG-OD1	5.21	122.99	118.30
1	E	8	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	82	ALA	N-CA-CB	-5.20	102.83	110.10
1	E	72	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	159	ASP	CA-CB-CG	-5.18	102.00	113.40
1	B	10	ASP	N-CA-C	5.18	124.97	111.00
1	C	70	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	9	ILE	CB-CA-C	-5.13	101.33	111.60
1	C	87	VAL	CA-CB-CG2	-5.12	103.21	110.90
1	D	18	TYR	CB-CG-CD1	5.10	124.06	121.00
1	E	80	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	E	25	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	70	ASP	CB-CG-OD2	-5.07	113.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	4	PHE	CB-CG-CD1	5.06	124.34	120.80
1	E	69	GLN	CB-CA-C	5.04	120.48	110.40

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	1289	0	1312	171	0
1	B	1289	0	1312	97	0
1	C	1289	0	1312	91	0
1	D	1289	0	1312	137	0
1	E	1289	0	1312	130	0
All	All	6445	0	6560	621	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 49.

All (621) 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:116:ASN:HA	1:D:119:ARG:HD2	1.34	1.08
1:E:53:ASN:ND2	1:E:53:ASN:H	1.46	1.07
1:A:116:ASN:HA	1:A:119:ARG:HD2	1.38	1.03
1:D:10:ASP:HB2	1:D:145:ARG:HG3	1.40	1.02
1:D:50:ILE:HD11	1:D:52:ARG:HG3	1.41	1.02
1:E:72:ASP:HB3	1:E:76:ARG:HH21	1.27	0.99
1:E:59:THR:HG23	1:E:62:GLU:HG3	1.46	0.98
1:A:95:ARG:NH1	1:A:156:GLY:HA3	1.85	0.92
1:E:53:ASN:N	1:E:53:ASN:HD22	1.67	0.91
1:C:16:LYS:HG2	1:C:57:VAL:HG22	1.51	0.91
1:B:59:THR:HG23	1:B:62:GLU:HG3	1.51	0.90
1:D:148:ARG:HG2	1:D:160:ALA:HB1	1.53	0.89
1:D:125:ARG:HB3	1:D:128:ALA:HB3	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HD21	1:D:112:ALA:HA	1.53	0.88
1:E:116:ASN:HA	1:E:119:ARG:CD	2.04	0.87
1:C:1:MET:HE2	1:C:5:GLU:HB3	1.56	0.87
1:D:116:ASN:HA	1:D:119:ARG:CD	2.04	0.87
1:A:52:ARG:NH1	1:A:54:CYS:HA	1.89	0.86
1:C:1:MET:CE	1:C:5:GLU:HB3	2.06	0.86
1:D:10:ASP:CB	1:D:145:ARG:HG3	2.05	0.85
1:B:116:ASN:HA	1:B:119:ARG:HD3	1.58	0.85
1:A:116:ASN:H	1:A:116:ASN:HD22	1.23	0.85
1:A:1:MET:CE	1:A:5:GLU:HB3	2.07	0.85
1:A:116:ASN:N	1:A:116:ASN:HD22	1.72	0.84
1:D:127:ASP:HA	1:D:130:ALA:CB	2.07	0.84
1:D:1:MET:HG2	1:D:158:TRP:CE3	2.12	0.84
1:B:103:VAL:HG23	1:B:111:VAL:HG21	1.59	0.83
1:A:151:THR:HG23	1:A:154:ARG:NH1	1.92	0.83
1:E:83:LYS:HD2	1:E:112:ALA:HB1	1.60	0.82
1:D:95:ARG:HH11	1:D:95:ARG:HG3	1.42	0.82
1:E:59:THR:HG23	1:E:62:GLU:CG	2.09	0.82
1:B:144:ASN:HD22	1:B:144:ASN:N	1.74	0.81
1:E:53:ASN:H	1:E:53:ASN:HD22	0.81	0.81
1:A:87:VAL:O	1:A:91:LEU:HG	1.81	0.81
1:B:4:PHE:HE2	1:B:60:LYS:HE2	1.44	0.80
1:D:116:ASN:CA	1:D:119:ARG:HD2	2.11	0.80
1:A:114:PHE:O	1:A:118:LEU:HG	1.81	0.80
1:A:115:THR:HG22	1:A:116:ASN:ND2	1.97	0.80
1:C:92:ASP:OD1	1:C:95:ARG:HG3	1.82	0.79
1:A:115:THR:HG22	1:A:116:ASN:HD22	1.46	0.79
1:A:116:ASN:HA	1:A:119:ARG:CD	2.13	0.79
1:D:120:MET:HB3	1:D:129:ALA:HB2	1.65	0.79
1:C:53:ASN:H	1:C:53:ASN:ND2	1.81	0.78
1:B:50:ILE:HD11	1:B:52:ARG:HG2	1.65	0.77
1:D:125:ARG:HB3	1:D:128:ALA:CB	2.15	0.77
1:D:1:MET:HA	1:D:1:MET:CE	2.15	0.77
1:E:99:LEU:O	1:E:103:VAL:HG12	1.83	0.77
1:E:116:ASN:HA	1:E:119:ARG:HD2	1.65	0.77
1:A:155:THR:OG1	1:A:157:THR:HG23	1.85	0.77
1:D:127:ASP:HA	1:D:130:ALA:HB3	1.66	0.77
1:A:16:LYS:HB3	1:A:16:LYS:NZ	2.00	0.77
1:E:137:ALA:O	1:E:141:GLN:HG2	1.84	0.76
1:E:124:LYS:HE2	1:E:126:TRP:HH2	1.50	0.76
1:D:127:ASP:HB3	1:D:154:ARG:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:LYS:HG3	1:B:66:LEU:N	1.99	0.76
1:D:43:LYS:HE2	1:D:55:ASN:OD1	1.85	0.76
1:A:59:THR:HG23	1:A:62:GLU:OE1	1.86	0.76
1:E:16:LYS:HG3	1:E:57:VAL:HG22	1.68	0.75
1:C:50:ILE:HG22	1:C:66:LEU:HD21	1.67	0.75
1:E:123:GLN:HB2	1:E:125:ARG:CD	2.17	0.74
1:C:47:ASP:OD1	1:C:54:CYS:HB2	1.86	0.74
1:E:59:THR:CG2	1:E:62:GLU:HG3	2.17	0.74
1:E:116:ASN:HA	1:E:119:ARG:HD3	1.67	0.74
1:A:2:ASN:OD1	1:A:5:GLU:HB2	1.88	0.74
1:E:124:LYS:HE2	1:E:126:TRP:CH2	2.22	0.74
1:B:123:GLN:HG3	1:B:125:ARG:CD	2.18	0.74
1:C:85:LYS:N	1:C:86:PRO:HD2	2.01	0.74
1:D:148:ARG:CG	1:D:160:ALA:HB1	2.17	0.74
1:E:123:GLN:HB2	1:E:125:ARG:HD2	1.69	0.74
1:D:137:ALA:O	1:D:141:GLN:HG2	1.88	0.74
1:A:151:THR:O	1:A:155:THR:HG23	1.88	0.73
1:A:74:ALA:O	1:A:78:ILE:HG13	1.87	0.73
1:D:50:ILE:O	1:D:50:ILE:HD12	1.89	0.73
1:B:1:MET:HG2	1:B:2:ASN:H	1.52	0.72
1:C:151:THR:O	1:C:155:THR:HG23	1.89	0.72
1:C:96:ARG:O	1:C:100:ILE:HD12	1.90	0.72
1:A:102:MET:CE	1:A:133:LEU:HD22	2.20	0.72
1:D:119:ARG:O	1:D:122:GLN:HB3	1.90	0.71
1:C:119:ARG:O	1:C:123:GLN:HG3	1.91	0.71
1:E:123:GLN:CB	1:E:125:ARG:HD2	2.22	0.70
1:E:85:LYS:HB3	1:E:86:PRO:HD3	1.72	0.70
1:A:1:MET:HE1	1:A:5:GLU:HB3	1.73	0.70
1:A:151:THR:HG23	1:A:154:ARG:HH12	1.55	0.70
1:E:88:TYR:CE1	1:E:96:ARG:HG2	2.27	0.70
1:D:129:ALA:O	1:D:132:ALA:HB3	1.91	0.70
1:C:50:ILE:HD11	1:C:52:ARG:HG2	1.72	0.70
1:E:27:ILE:HD12	1:E:46:LEU:CD2	2.22	0.70
1:E:14:ARG:HG3	1:E:18:TYR:CE1	2.27	0.69
1:E:94:VAL:O	1:E:97:CYS:HB2	1.92	0.69
1:B:13:LEU:HD12	1:B:29:ILE:CG1	2.22	0.69
1:A:3:ILE:CD1	1:A:97:CYS:HA	2.22	0.69
1:B:123:GLN:HG3	1:B:125:ARG:HD3	1.74	0.69
1:E:91:LEU:HD22	1:E:95:ARG:HB3	1.72	0.69
1:D:84:LEU:O	1:D:87:VAL:HG23	1.94	0.68
1:D:113:GLY:O	1:D:115:THR:N	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:VAL:HG22	1:A:111:VAL:HG21	1.75	0.68
1:A:1:MET:HB3	1:A:158:TRP:CD1	2.29	0.68
1:A:102:MET:HE3	1:A:138:TRP:CH2	2.29	0.68
1:C:137:ALA:C	1:C:141:GLN:HE21	1.96	0.68
1:C:2:ASN:HD21	1:C:4:PHE:HB3	1.59	0.68
1:A:52:ARG:HH12	1:A:54:CYS:HA	1.59	0.67
1:B:74:ALA:O	1:B:78:ILE:HG13	1.94	0.67
1:D:50:ILE:CD1	1:D:52:ARG:HG3	2.22	0.67
1:D:127:ASP:HA	1:D:130:ALA:HB2	1.75	0.67
1:C:33:LEU:HD21	1:C:46:LEU:HD13	1.77	0.67
1:A:7:LEU:HD13	1:A:67:PHE:CE1	2.29	0.67
1:D:1:MET:HE2	1:D:1:MET:HA	1.76	0.67
1:A:115:THR:HG22	1:A:116:ASN:N	2.10	0.66
1:D:139:TYR:CE2	1:D:147:LYS:HG3	2.30	0.66
1:B:1:MET:CG	1:B:2:ASN:H	2.07	0.66
1:E:59:THR:HG23	1:E:62:GLU:CD	2.15	0.66
1:A:36:SER:O	1:A:38:SER:N	2.29	0.66
1:C:13:LEU:O	1:C:14:ARG:HG3	1.96	0.66
1:E:7:LEU:HD13	1:E:67:PHE:HZ	1.60	0.66
1:D:116:ASN:O	1:D:119:ARG:HD2	1.95	0.66
1:A:46:LEU:O	1:A:49:ALA:HB3	1.96	0.66
1:E:89:ASP:HA	1:E:96:ARG:HH21	1.60	0.66
1:A:92:ASP:O	1:A:94:VAL:N	2.29	0.66
1:B:13:LEU:HD12	1:B:29:ILE:HG13	1.78	0.66
1:A:54:CYS:HB3	1:A:57:VAL:O	1.95	0.65
1:B:92:ASP:OD1	1:B:95:ARG:HG3	1.96	0.65
1:B:45:GLU:OE1	1:B:45:GLU:HA	1.96	0.65
1:E:59:THR:OG1	1:E:61:ASP:N	2.29	0.65
1:D:140:ASN:O	1:D:143:PRO:HD3	1.97	0.65
1:A:10:ASP:OD1	1:A:148:ARG:NH2	2.29	0.65
1:A:84:LEU:C	1:A:86:PRO:HD2	2.16	0.65
1:A:2:ASN:OD1	1:A:2:ASN:N	2.29	0.65
1:D:103:VAL:HG23	1:D:111:VAL:HG21	1.79	0.65
1:A:71:VAL:O	1:A:75:VAL:HG23	1.97	0.65
1:C:27:ILE:HD13	1:C:58:ILE:HD13	1.77	0.64
1:C:72:ASP:HB3	1:C:76:ARG:NH2	2.12	0.64
1:D:26:THR:HG22	1:D:27:ILE:N	2.13	0.64
1:E:53:ASN:ND2	1:E:53:ASN:N	2.28	0.64
1:D:125:ARG:O	1:D:128:ALA:HB3	1.97	0.64
1:B:60:LYS:HZ2	1:B:60:LYS:HB3	1.62	0.64
1:C:4:PHE:CE1	1:C:29:ILE:HD11	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:TYR:CZ	1:D:96:ARG:HD3	2.32	0.64
1:E:7:LEU:HD13	1:E:67:PHE:CZ	2.32	0.64
1:B:59:THR:HG23	1:B:62:GLU:CG	2.25	0.64
1:E:100:ILE:HA	1:E:103:VAL:CG1	2.28	0.64
1:B:79:LEU:HD11	1:C:35:LYS:HD3	1.80	0.64
1:A:102:MET:HE1	1:A:133:LEU:HD22	1.79	0.64
1:A:102:MET:HB3	1:A:111:VAL:CG1	2.29	0.63
1:E:72:ASP:CB	1:E:76:ARG:HH21	2.09	0.63
1:B:144:ASN:ND2	1:B:144:ASN:N	2.45	0.63
1:C:50:ILE:C	1:C:50:ILE:HD12	2.18	0.63
1:B:72:ASP:OD1	1:C:36:SER:HB2	1.98	0.63
1:A:81:ASN:ND2	1:A:108:GLU:OE1	2.30	0.63
1:A:105:GLN:HB2	1:A:145:ARG:NH2	2.14	0.63
1:E:58:ILE:HB	1:E:62:GLU:HB2	1.79	0.63
1:D:84:LEU:HA	1:D:87:VAL:CG2	2.29	0.63
1:A:87:VAL:CG2	1:A:122:GLN:HG3	2.29	0.62
1:A:6:MET:HE2	1:A:101:ASN:HB2	1.81	0.62
1:E:27:ILE:HD11	1:E:58:ILE:HG12	1.81	0.62
1:A:52:ARG:HG3	1:A:53:ASN:N	2.13	0.62
1:E:58:ILE:HG22	1:E:62:GLU:OE1	1.99	0.62
1:A:16:LYS:HZ3	1:A:16:LYS:HB3	1.63	0.62
1:A:113:GLY:O	1:A:115:THR:N	2.33	0.62
1:D:8:ARG:O	1:D:12:GLY:HA2	2.00	0.62
1:D:13:LEU:HD21	1:D:60:LYS:HG2	1.81	0.62
1:D:95:ARG:HH11	1:D:95:ARG:CG	2.12	0.62
1:A:16:LYS:HG3	1:A:56:GLY:O	1.99	0.62
1:A:85:LYS:HB3	1:A:86:PRO:HD3	1.81	0.62
1:E:115:THR:O	1:E:119:ARG:HG3	1.99	0.62
1:B:115:THR:HG22	1:B:116:ASN:N	2.14	0.62
1:C:46:LEU:O	1:C:49:ALA:N	2.32	0.62
1:A:110:GLY:O	1:A:113:GLY:N	2.29	0.61
1:E:27:ILE:HD12	1:E:46:LEU:HD22	1.82	0.61
1:A:124:LYS:HB3	1:A:126:TRP:CZ2	2.35	0.61
1:E:124:LYS:HA	1:E:126:TRP:CH2	2.34	0.61
1:D:139:TYR:HE2	1:D:147:LYS:HG3	1.65	0.61
1:A:3:ILE:HD12	1:A:97:CYS:CB	2.30	0.61
1:D:7:LEU:HD11	1:D:101:ASN:HB2	1.82	0.61
1:B:96:ARG:O	1:B:100:ILE:N	2.31	0.61
1:A:87:VAL:HG22	1:A:122:GLN:HG3	1.82	0.61
1:C:24:TYR:CE2	1:C:35:LYS:HE2	2.36	0.61
1:A:116:ASN:ND2	1:A:116:ASN:N	2.45	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:THR:HG22	1:E:27:ILE:N	2.15	0.61
1:E:155:THR:O	1:E:157:THR:HG23	2.00	0.61
1:C:50:ILE:HD11	1:C:54:CYS:SG	2.41	0.61
1:A:47:ASP:O	1:A:51:GLY:HA2	2.01	0.60
1:E:59:THR:HG1	1:E:62:GLU:H	1.49	0.60
1:B:115:THR:CG2	1:B:119:ARG:HD2	2.30	0.60
1:B:50:ILE:CD1	1:B:52:ARG:HG2	2.30	0.60
1:B:16:LYS:HG3	1:B:57:VAL:HG22	1.83	0.60
1:A:18:TYR:O	1:A:26:THR:N	2.30	0.60
1:D:115:THR:O	1:D:119:ARG:HG3	2.01	0.60
1:C:124:LYS:HD3	1:C:126:TRP:HZ2	1.67	0.60
1:C:60:LYS:O	1:C:63:ALA:HB3	2.02	0.59
1:B:115:THR:HG23	1:B:119:ARG:HD2	1.83	0.59
1:B:123:GLN:HG3	1:B:125:ARG:NE	2.17	0.59
1:A:95:ARG:HH12	1:A:156:GLY:HA3	1.64	0.59
1:D:114:PHE:CD2	1:D:133:LEU:HD23	2.36	0.59
1:E:125:ARG:NH1	1:E:125:ARG:HG2	2.18	0.59
1:A:107:GLY:O	1:A:111:VAL:HG22	2.01	0.59
1:D:67:PHE:O	1:D:71:VAL:HG23	2.02	0.59
1:B:18:TYR:CZ	1:B:26:THR:HG22	2.38	0.59
1:A:7:LEU:HD13	1:A:67:PHE:HE1	1.67	0.59
1:D:66:LEU:O	1:D:69:GLN:HB2	2.03	0.59
1:A:3:ILE:HD12	1:A:97:CYS:HB3	1.84	0.59
1:D:84:LEU:HA	1:D:87:VAL:HG23	1.82	0.59
1:B:50:ILE:O	1:B:50:ILE:HD12	2.03	0.59
1:B:46:LEU:O	1:B:49:ALA:N	2.36	0.59
1:E:100:ILE:HD12	1:E:100:ILE:N	2.18	0.58
1:B:155:THR:OG1	1:B:157:THR:HG23	2.04	0.58
1:E:75:VAL:HG12	1:E:79:LEU:HD12	1.85	0.58
1:D:50:ILE:HD11	1:D:54:CYS:SG	2.43	0.58
1:A:50:ILE:HD11	1:A:54:CYS:SG	2.44	0.58
1:E:114:PHE:O	1:E:118:LEU:HG	2.03	0.57
1:E:4:PHE:HE2	1:E:60:LYS:HZ2	1.52	0.57
1:A:100:ILE:O	1:A:104:PHE:N	2.34	0.57
1:A:102:MET:HE2	1:A:133:LEU:HD22	1.85	0.57
1:D:87:VAL:O	1:D:90:SER:HB3	2.05	0.57
1:B:120:MET:HE3	1:B:129:ALA:N	2.20	0.57
1:C:120:MET:HG2	1:C:125:ARG:HD3	1.86	0.57
1:E:90:SER:OG	1:E:124:LYS:HE3	2.04	0.57
1:A:52:ARG:HG2	1:A:54:CYS:SG	2.44	0.57
1:B:123:GLN:CG	1:B:125:ARG:HD3	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:LEU:HD21	1:D:112:ALA:CA	2.31	0.57
1:C:137:ALA:HB1	1:C:141:GLN:NE2	2.20	0.57
1:B:88:TYR:CE1	1:B:96:ARG:HD3	2.39	0.57
1:A:116:ASN:ND2	1:A:116:ASN:H	1.99	0.57
1:B:7:LEU:HD13	1:B:67:PHE:CZ	2.39	0.57
1:E:46:LEU:C	1:E:46:LEU:HD12	2.25	0.56
1:D:17:ILE:HG22	1:D:18:TYR:N	2.20	0.56
1:D:114:PHE:HD1	1:D:114:PHE:H	1.52	0.56
1:D:116:ASN:C	1:D:119:ARG:HD2	2.24	0.56
1:D:7:LEU:HD23	1:D:11:GLU:HG3	1.87	0.56
1:C:24:TYR:HB3	1:C:32:LEU:CD1	2.35	0.56
1:B:7:LEU:HD13	1:B:67:PHE:CE1	2.39	0.56
1:A:116:ASN:CA	1:A:119:ARG:HD2	2.26	0.56
1:D:1:MET:HG3	1:D:2:ASN:N	2.20	0.56
1:A:10:ASP:HB3	1:A:145:ARG:HD2	1.86	0.56
1:A:1:MET:HB3	1:A:158:TRP:CG	2.39	0.56
1:B:50:ILE:HD11	1:B:54:CYS:SG	2.45	0.56
1:D:116:ASN:HA	1:D:119:ARG:NE	2.20	0.56
1:B:13:LEU:HD12	1:B:29:ILE:HG12	1.88	0.56
1:C:92:ASP:O	1:C:96:ARG:HG3	2.07	0.55
1:A:96:ARG:NH1	1:B:24:TYR:CE1	2.73	0.55
1:A:60:LYS:HD2	1:A:60:LYS:O	2.06	0.55
1:A:106:MET:HE2	1:A:138:TRP:CD1	2.41	0.55
1:E:32:LEU:HD11	1:E:35:LYS:HG3	1.89	0.55
1:A:17:ILE:CD1	1:A:43:LYS:HG3	2.37	0.55
1:A:67:PHE:CE2	1:A:71:VAL:HG21	2.42	0.55
1:D:143:PRO:O	1:D:147:LYS:N	2.36	0.55
1:C:25:TYR:CZ	1:C:39:LEU:HD13	2.41	0.55
1:D:1:MET:HE2	1:D:5:GLU:HB2	1.88	0.55
1:E:5:GLU:OE1	1:E:8:ARG:NE	2.29	0.55
1:E:94:VAL:HG22	1:E:158:TRP:CE2	2.42	0.55
1:E:59:THR:HG1	1:E:61:ASP:HB2	1.72	0.55
1:A:45:GLU:O	1:A:49:ALA:HB2	2.07	0.55
1:D:120:MET:CB	1:D:129:ALA:HB2	2.36	0.54
1:B:121:LEU:HD23	1:B:129:ALA:CB	2.38	0.54
1:A:8:ARG:O	1:A:12:GLY:HA2	2.07	0.54
1:A:8:ARG:NH2	1:A:9:ILE:HG13	2.22	0.54
1:B:88:TYR:CZ	1:B:96:ARG:HD3	2.43	0.54
1:D:83:LYS:O	1:D:86:PRO:HD2	2.07	0.54
1:E:66:LEU:O	1:E:69:GLN:HG3	2.08	0.54
1:C:26:THR:HG22	1:C:27:ILE:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:GLU:HG2	1:D:145:ARG:NH2	2.22	0.54
1:A:155:THR:OG1	1:A:156:GLY:N	2.39	0.54
1:D:1:MET:HE2	1:D:5:GLU:CB	2.37	0.54
1:C:87:VAL:O	1:C:90:SER:HB3	2.07	0.54
1:A:92:ASP:OD2	1:A:95:ARG:HD2	2.08	0.54
1:E:58:ILE:HA	1:E:62:GLU:OE1	2.08	0.54
1:C:5:GLU:OE1	1:C:8:ARG:NH2	2.38	0.54
1:E:105:GLN:HG2	1:E:106:MET:HE3	1.90	0.54
1:C:143:PRO:O	1:C:147:LYS:HG3	2.06	0.54
1:D:139:TYR:OH	1:D:147:LYS:NZ	2.37	0.54
1:B:106:MET:O	1:B:110:GLY:HA3	2.08	0.54
1:C:114:PHE:O	1:C:118:LEU:HG	2.08	0.54
1:A:6:MET:SD	1:A:158:TRP:HZ3	2.31	0.53
1:B:24:TYR:CE1	1:B:35:LYS:HG2	2.43	0.53
1:B:52:ARG:NH1	1:B:54:CYS:HA	2.22	0.53
1:B:120:MET:CE	1:B:128:ALA:HB1	2.38	0.53
1:A:32:LEU:HD23	1:A:34:THR:N	2.23	0.53
1:E:77:GLY:HA2	1:E:80:ARG:CZ	2.38	0.53
1:B:1:MET:CG	1:B:2:ASN:N	2.72	0.53
1:A:100:ILE:HG22	1:A:104:PHE:CD1	2.44	0.53
1:A:144:ASN:O	1:A:147:LYS:N	2.40	0.53
1:B:60:LYS:NZ	1:B:60:LYS:HB3	2.21	0.53
1:A:72:ASP:HB3	1:A:76:ARG:HH21	1.73	0.53
1:A:1:MET:HE3	1:A:6:MET:N	2.24	0.53
1:D:105:GLN:HB2	1:D:145:ARG:NH2	2.24	0.53
1:B:8:ARG:CZ	1:B:9:ILE:HD12	2.38	0.53
1:C:1:MET:HE3	1:C:5:GLU:HB3	1.90	0.53
1:A:24:TYR:OH	1:E:96:ARG:NH2	2.41	0.53
1:D:19:LYS:HA	1:D:24:TYR:O	2.09	0.53
1:B:60:LYS:C	1:B:60:LYS:HZ3	2.12	0.53
1:E:32:LEU:C	1:E:32:LEU:HD23	2.29	0.53
1:E:60:LYS:O	1:E:63:ALA:HB3	2.09	0.53
1:C:106:MET:CE	1:C:138:TRP:CD1	2.91	0.53
1:C:155:THR:OG1	1:C:157:THR:HG23	2.09	0.53
1:A:5:GLU:OE1	1:A:8:ARG:NE	2.41	0.52
1:D:50:ILE:C	1:D:50:ILE:HD12	2.30	0.52
1:C:106:MET:HE3	1:C:138:TRP:CD1	2.44	0.52
1:A:120:MET:HB2	1:A:129:ALA:HB2	1.90	0.52
1:D:148:ARG:HG2	1:D:160:ALA:CB	2.31	0.52
1:E:119:ARG:O	1:E:123:GLN:HG2	2.10	0.52
1:B:4:PHE:CE1	1:B:64:GLU:HA	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LEU:HD23	1:B:129:ALA:HB1	1.91	0.52
1:A:79:LEU:C	1:A:81:ASN:H	2.13	0.52
1:D:119:ARG:O	1:D:123:GLN:HG2	2.08	0.52
1:A:106:MET:CE	1:A:138:TRP:CD1	2.93	0.52
1:E:125:ARG:HG2	1:E:125:ARG:HH11	1.73	0.52
1:D:22:GLU:HB2	1:D:24:TYR:CD2	2.45	0.52
1:A:92:ASP:O	1:A:95:ARG:N	2.42	0.52
1:E:4:PHE:HE2	1:E:60:LYS:NZ	2.08	0.52
1:C:124:LYS:HD3	1:C:126:TRP:CZ2	2.45	0.51
1:B:130:ALA:CB	1:B:154:ARG:HG3	2.40	0.51
1:C:75:VAL:CG1	1:C:79:LEU:HD11	2.40	0.51
1:D:85:LYS:N	1:D:86:PRO:HD2	2.25	0.51
1:A:137:ALA:O	1:A:141:GLN:HG2	2.10	0.51
1:A:4:PHE:CE2	1:A:64:GLU:HG3	2.44	0.51
1:D:1:MET:HB3	1:D:158:TRP:CG	2.44	0.51
1:E:89:ASP:HA	1:E:96:ARG:NH2	2.25	0.51
1:E:124:LYS:HA	1:E:126:TRP:CZ3	2.45	0.51
1:A:18:TYR:CE1	1:A:26:THR:HG22	2.45	0.51
1:D:87:VAL:O	1:D:90:SER:N	2.42	0.51
1:D:91:LEU:HB2	1:D:96:ARG:HG2	1.92	0.51
1:C:50:ILE:CD1	1:C:52:ARG:HG2	2.38	0.51
1:E:103:VAL:O	1:E:107:GLY:N	2.43	0.51
1:C:120:MET:CG	1:C:125:ARG:HD3	2.39	0.51
1:D:22:GLU:HB2	1:D:24:TYR:HD2	1.75	0.51
1:D:26:THR:CG2	1:D:27:ILE:N	2.74	0.51
1:B:81:ASN:OD1	1:B:83:LYS:N	2.39	0.51
1:D:60:LYS:O	1:D:63:ALA:HB3	2.11	0.50
1:E:100:ILE:HD12	1:E:100:ILE:H	1.76	0.50
1:E:96:ARG:O	1:E:100:ILE:HD12	2.10	0.50
1:C:85:LYS:HB3	1:C:86:PRO:HD3	1.93	0.50
1:E:13:LEU:HD21	1:E:60:LYS:HG2	1.92	0.50
1:D:85:LYS:N	1:D:86:PRO:CD	2.74	0.50
1:A:118:LEU:HD23	1:A:118:LEU:N	2.27	0.50
1:B:71:VAL:HG11	1:C:36:SER:OG	2.11	0.50
1:B:120:MET:SD	1:B:128:ALA:HB1	2.52	0.50
1:A:137:ALA:O	1:A:140:ASN:N	2.43	0.50
1:D:52:ARG:NH1	1:D:54:CYS:HA	2.26	0.50
1:A:7:LEU:O	1:A:11:GLU:N	2.42	0.50
1:E:76:ARG:HB3	1:E:80:ARG:NH1	2.26	0.50
1:B:26:THR:CG2	1:B:27:ILE:N	2.74	0.50
1:E:105:GLN:HG2	1:E:106:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ALA:O	1:B:140:ASN:N	2.40	0.50
1:A:85:LYS:N	1:A:86:PRO:HD2	2.27	0.50
1:C:76:ARG:O	1:C:80:ARG:HG3	2.12	0.50
1:A:100:ILE:HG22	1:A:104:PHE:HD1	1.77	0.50
1:D:138:TRP:HA	1:D:141:GLN:HG3	1.93	0.50
1:A:73:ALA:HA	1:A:76:ARG:NH1	2.27	0.50
1:B:138:TRP:CZ2	1:B:146:ALA:HA	2.47	0.50
1:A:29:ILE:O	1:A:29:ILE:HG22	2.10	0.49
1:A:125:ARG:HB3	1:A:128:ALA:HB3	1.94	0.49
1:A:1:MET:HB3	1:A:158:TRP:CE2	2.47	0.49
1:E:81:ASN:HB3	1:E:84:LEU:HB2	1.94	0.49
1:D:139:TYR:CZ	1:D:147:LYS:NZ	2.80	0.49
1:E:72:ASP:HB3	1:E:76:ARG:NH2	2.11	0.49
1:B:50:ILE:C	1:B:50:ILE:HD12	2.33	0.49
1:A:65:LYS:HG3	1:A:66:LEU:N	2.26	0.49
1:E:120:MET:HE3	1:E:129:ALA:N	2.28	0.49
1:B:2:ASN:N	1:B:2:ASN:OD1	2.45	0.49
1:B:85:LYS:HE3	1:B:89:ASP:OD2	2.12	0.49
1:C:6:MET:CE	1:C:158:TRP:HZ3	2.26	0.49
1:A:47:ASP:OD1	1:A:52:ARG:O	2.30	0.49
1:A:85:LYS:CB	1:A:86:PRO:HD3	2.42	0.49
1:B:18:TYR:O	1:B:26:THR:N	2.40	0.49
1:E:115:THR:HG22	1:E:116:ASN:N	2.28	0.49
1:C:13:LEU:HD11	1:C:63:ALA:HB1	1.94	0.49
1:D:26:THR:HG23	1:D:31:HIS:O	2.12	0.49
1:E:91:LEU:HA	1:E:124:LYS:HZ1	1.77	0.49
1:D:1:MET:HE3	1:D:1:MET:HA	1.95	0.48
1:E:1:MET:HE1	1:E:5:GLU:HB3	1.94	0.48
1:B:18:TYR:CE1	1:B:26:THR:HG22	2.49	0.48
1:D:20:ASP:N	1:D:24:TYR:O	2.45	0.48
1:A:1:MET:HB3	1:A:158:TRP:CD2	2.48	0.48
1:E:50:ILE:HD13	1:E:62:GLU:CD	2.32	0.48
1:E:125:ARG:CG	1:E:125:ARG:HH11	2.23	0.48
1:E:5:GLU:O	1:E:9:ILE:HG13	2.13	0.48
1:B:39:LEU:HG	1:B:39:LEU:O	2.13	0.48
1:E:120:MET:HA	1:E:123:GLN:HG3	1.95	0.48
1:E:3:ILE:HG23	1:E:4:PHE:N	2.27	0.48
1:A:144:ASN:O	1:A:147:LYS:HB2	2.14	0.48
1:A:81:ASN:CG	1:A:84:LEU:HD12	2.33	0.48
1:D:33:LEU:O	1:D:34:THR:HB	2.14	0.48
1:E:27:ILE:HD13	1:E:58:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:TYR:CZ	1:D:147:LYS:CE	2.97	0.48
1:D:31:HIS:HD2	1:D:33:LEU:HD23	1.77	0.48
1:D:60:LYS:HB3	1:D:60:LYS:NZ	2.28	0.48
1:A:94:VAL:CG1	1:A:95:ARG:N	2.78	0.47
1:E:115:THR:HG22	1:E:119:ARG:HD2	1.95	0.47
1:B:94:VAL:O	1:B:97:CYS:HB2	2.14	0.47
1:A:108:GLU:O	1:A:112:ALA:N	2.29	0.47
1:C:16:LYS:CG	1:C:57:VAL:HG22	2.36	0.47
1:C:1:MET:HG3	1:C:2:ASN:N	2.29	0.47
1:A:142:THR:O	1:A:146:ALA:HB3	2.14	0.47
1:C:16:LYS:HG2	1:C:57:VAL:CG2	2.33	0.47
1:A:50:ILE:HD12	1:A:58:ILE:HG22	1.96	0.47
1:B:127:ASP:OD1	1:B:154:ARG:NE	2.47	0.47
1:D:139:TYR:CZ	1:D:147:LYS:HE2	2.49	0.47
1:E:1:MET:CG	1:E:2:ASN:N	2.77	0.47
1:A:26:THR:CG2	1:A:27:ILE:N	2.77	0.47
1:E:124:LYS:HB3	1:E:126:TRP:CZ2	2.49	0.47
1:B:33:LEU:HD23	1:B:33:LEU:HA	1.51	0.47
1:B:103:VAL:CG2	1:B:111:VAL:HG21	2.38	0.47
1:A:16:LYS:C	1:A:27:ILE:HD12	2.35	0.47
1:E:1:MET:HG3	1:E:2:ASN:N	2.29	0.47
1:B:79:LEU:C	1:B:81:ASN:H	2.18	0.47
1:B:18:TYR:CZ	1:B:26:THR:CG2	2.98	0.47
1:E:143:PRO:HB2	1:E:147:LYS:HZ3	1.80	0.47
1:B:139:TYR:CZ	1:B:147:LYS:HE2	2.50	0.47
1:B:38:SER:OG	1:B:41:ALA:N	2.29	0.47
1:A:116:ASN:HA	1:A:119:ARG:HG3	1.97	0.47
1:E:26:THR:HG23	1:E:31:HIS:C	2.36	0.47
1:D:84:LEU:C	1:D:87:VAL:HG23	2.36	0.47
1:D:140:ASN:C	1:D:143:PRO:HD3	2.35	0.47
1:A:3:ILE:CG2	1:A:4:PHE:N	2.77	0.46
1:D:93:ALA:O	1:D:96:ARG:N	2.47	0.46
1:C:72:ASP:HB3	1:C:76:ARG:HH22	1.78	0.46
1:B:85:LYS:HB3	1:B:86:PRO:HD3	1.97	0.46
1:B:5:GLU:O	1:B:8:ARG:HB3	2.15	0.46
1:C:26:THR:HG23	1:C:31:HIS:O	2.15	0.46
1:D:13:LEU:HD21	1:D:60:LYS:CG	2.45	0.46
1:A:119:ARG:O	1:A:122:GLN:HB2	2.14	0.46
1:D:7:LEU:O	1:D:11:GLU:HB2	2.15	0.46
1:A:15:LEU:O	1:A:57:VAL:HG13	2.15	0.46
1:B:87:VAL:HG21	1:B:118:LEU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ALA:O	1:C:150:ILE:HG13	2.15	0.46
1:A:115:THR:CG2	1:A:119:ARG:NH1	2.78	0.46
1:A:85:LYS:N	1:A:86:PRO:CD	2.79	0.46
1:E:59:THR:HG1	1:E:61:ASP:CB	2.27	0.46
1:C:26:THR:HG21	1:C:30:GLY:HA2	1.97	0.46
1:E:10:ASP:OD1	1:E:145:ARG:HG3	2.15	0.46
1:A:138:TRP:HA	1:A:141:GLN:HG3	1.96	0.46
1:C:13:LEU:HD13	1:C:29:ILE:CG1	2.46	0.46
1:E:85:LYS:N	1:E:86:PRO:CD	2.78	0.46
1:A:87:VAL:HG23	1:A:122:GLN:HG3	1.98	0.46
1:D:84:LEU:C	1:D:86:PRO:HD2	2.36	0.46
1:B:17:ILE:CG2	1:B:18:TYR:N	2.78	0.46
1:A:116:ASN:HA	1:A:119:ARG:CG	2.45	0.46
1:A:85:LYS:HB3	1:A:86:PRO:CD	2.44	0.46
1:D:105:GLN:HG3	1:D:145:ARG:CZ	2.46	0.46
1:D:17:ILE:CG2	1:D:18:TYR:N	2.79	0.46
1:A:102:MET:CE	1:A:138:TRP:CH2	2.98	0.46
1:D:9:ILE:HG22	1:D:148:ARG:NH1	2.30	0.46
1:A:6:MET:CE	1:A:101:ASN:HB2	2.43	0.46
1:E:92:ASP:OD2	1:E:95:ARG:NH1	2.48	0.46
1:E:1:MET:HB3	1:E:158:TRP:CG	2.51	0.46
1:E:81:ASN:OD1	1:E:83:LYS:N	2.42	0.45
1:E:137:ALA:O	1:E:140:ASN:HB2	2.16	0.45
1:B:121:LEU:CD2	1:B:129:ALA:HB1	2.46	0.45
1:A:124:LYS:HA	1:A:126:TRP:CH2	2.51	0.45
1:C:2:ASN:ND2	1:C:4:PHE:H	2.13	0.45
1:B:4:PHE:HE2	1:B:60:LYS:CE	2.20	0.45
1:C:75:VAL:HG12	1:C:79:LEU:CD1	2.47	0.45
1:D:92:ASP:O	1:D:96:ARG:N	2.48	0.45
1:A:63:ALA:HA	1:A:66:LEU:HD12	1.99	0.45
1:B:48:LYS:HE2	1:B:48:LYS:HB3	1.48	0.45
1:A:26:THR:HG22	1:A:27:ILE:N	2.30	0.45
1:D:139:TYR:HA	1:D:146:ALA:CB	2.47	0.45
1:D:137:ALA:O	1:D:140:ASN:HB2	2.17	0.45
1:E:14:ARG:HG3	1:E:18:TYR:CD1	2.52	0.45
1:E:1:MET:CE	1:E:5:GLU:HB3	2.47	0.45
1:E:79:LEU:HD23	1:E:79:LEU:HA	1.89	0.45
1:A:3:ILE:HG23	1:A:67:PHE:CE2	2.52	0.45
1:C:24:TYR:CE2	1:C:35:LYS:CE	2.99	0.45
1:D:24:TYR:HB3	1:D:32:LEU:HD12	1.99	0.45
1:E:26:THR:CG2	1:E:27:ILE:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:N	1:D:143:PRO:CD	2.79	0.45
1:B:5:GLU:O	1:B:8:ARG:N	2.47	0.45
1:C:20:ASP:OD1	1:C:22:GLU:N	2.50	0.45
1:B:91:LEU:HA	1:B:91:LEU:HD23	1.56	0.45
1:A:18:TYR:CZ	1:A:26:THR:HG22	2.51	0.45
1:C:137:ALA:CB	1:C:141:GLN:HE21	2.28	0.45
1:D:83:LYS:O	1:D:86:PRO:HG2	2.17	0.45
1:C:4:PHE:HA	1:C:67:PHE:CE2	2.51	0.45
1:D:138:TRP:CZ2	1:D:146:ALA:HA	2.52	0.45
1:C:26:THR:HG22	1:C:27:ILE:N	2.32	0.45
1:A:34:THR:OG1	1:A:35:LYS:N	2.50	0.45
1:A:78:ILE:CD1	1:A:103:VAL:HG21	2.46	0.45
1:A:105:GLN:HE22	1:A:138:TRP:HD1	1.64	0.45
1:A:7:LEU:HD12	1:A:67:PHE:HZ	1.82	0.45
1:A:8:ARG:NH2	1:A:9:ILE:HD11	2.31	0.45
1:D:60:LYS:HZ2	1:D:60:LYS:CB	2.29	0.44
1:E:8:ARG:O	1:E:12:GLY:N	2.48	0.44
1:C:39:LEU:O	1:C:43:LYS:HB2	2.17	0.44
1:A:98:ALA:HB2	1:A:152:THR:HG22	2.00	0.44
1:A:45:GLU:OE1	1:A:45:GLU:HA	2.17	0.44
1:D:29:ILE:O	1:D:29:ILE:HG22	2.17	0.44
1:A:65:LYS:O	1:A:69:GLN:HG3	2.17	0.44
1:E:24:TYR:HD1	1:E:24:TYR:HA	1.61	0.44
1:A:137:ALA:CB	1:A:141:GLN:HE21	2.30	0.44
1:C:155:THR:O	1:C:157:THR:HG23	2.17	0.44
1:E:52:ARG:O	1:E:54:CYS:N	2.50	0.44
1:E:120:MET:HE3	1:E:128:ALA:C	2.37	0.44
1:C:59:THR:OG1	1:C:62:GLU:HG3	2.18	0.44
1:A:6:MET:SD	1:A:158:TRP:CZ3	3.11	0.44
1:A:71:VAL:O	1:A:74:ALA:HB3	2.17	0.44
1:D:105:GLN:HG3	1:D:145:ARG:NH1	2.33	0.44
1:B:115:THR:HG22	1:B:119:ARG:CD	2.47	0.44
1:D:60:LYS:HZ2	1:D:60:LYS:C	2.21	0.44
1:A:32:LEU:C	1:A:32:LEU:HD23	2.38	0.44
1:D:123:GLN:O	1:D:124:LYS:HB2	2.18	0.44
1:A:6:MET:CE	1:A:101:ASN:HD22	2.31	0.44
1:E:59:THR:OG1	1:E:61:ASP:HB2	2.18	0.44
1:E:120:MET:HE3	1:E:129:ALA:CA	2.48	0.44
1:C:8:ARG:O	1:C:12:GLY:HA2	2.17	0.44
1:D:139:TYR:CE2	1:D:147:LYS:HE2	2.53	0.44
1:D:26:THR:HG22	1:D:27:ILE:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:GLN:H	1:A:123:GLN:HG2	1.31	0.44
1:A:7:LEU:HD13	1:A:67:PHE:CZ	2.52	0.44
1:A:8:ARG:NH2	1:A:9:ILE:CG1	2.81	0.44
1:A:72:ASP:HB3	1:A:76:ARG:NH2	2.32	0.44
1:D:79:LEU:HA	1:D:79:LEU:HD23	1.77	0.44
1:E:26:THR:HG22	1:E:27:ILE:H	1.80	0.43
1:E:46:LEU:HD23	1:E:56:GLY:HA2	1.99	0.43
1:D:1:MET:HG3	1:D:2:ASN:H	1.83	0.43
1:A:32:LEU:CD2	1:A:34:THR:N	2.81	0.43
1:E:76:ARG:HB3	1:E:80:ARG:HH12	1.83	0.43
1:D:95:ARG:HD3	1:D:153:PHE:HA	2.00	0.43
1:C:137:ALA:HB1	1:C:141:GLN:HE21	1.82	0.43
1:C:19:LYS:HA	1:C:24:TYR:O	2.19	0.43
1:C:36:SER:OG	1:C:37:PRO:HD2	2.18	0.43
1:A:73:ALA:HA	1:A:76:ARG:CZ	2.49	0.43
1:B:122:GLN:C	1:B:124:LYS:H	2.20	0.43
1:E:26:THR:HG23	1:E:31:HIS:O	2.18	0.43
1:E:1:MET:HG3	1:E:2:ASN:H	1.83	0.43
1:C:130:ALA:CB	1:C:154:ARG:HG3	2.49	0.43
1:A:7:LEU:CD1	1:A:67:PHE:CZ	3.01	0.43
1:D:95:ARG:CG	1:D:95:ARG:NH1	2.78	0.43
1:E:1:MET:CG	1:E:2:ASN:H	2.31	0.43
1:D:60:LYS:CB	1:D:60:LYS:NZ	2.77	0.43
1:E:133:LEU:HD23	1:E:133:LEU:HA	1.46	0.43
1:A:81:ASN:ND2	1:A:108:GLU:HB3	2.34	0.43
1:E:120:MET:HB3	1:E:125:ARG:HD3	2.01	0.43
1:C:13:LEU:HD13	1:C:29:ILE:HG12	2.00	0.43
1:D:84:LEU:HD22	1:D:111:VAL:HG12	2.01	0.43
1:A:50:ILE:CD1	1:A:58:ILE:HG22	2.49	0.43
1:B:17:ILE:HG12	1:B:33:LEU:HD12	2.01	0.43
1:A:27:ILE:HG13	1:A:28:GLY:N	2.33	0.43
1:A:61:ASP:O	1:A:64:GLU:HB3	2.19	0.43
1:B:60:LYS:O	1:B:63:ALA:HB3	2.19	0.43
1:E:100:ILE:O	1:E:103:VAL:HG13	2.19	0.43
1:B:13:LEU:CD1	1:B:29:ILE:HG13	2.48	0.43
1:D:114:PHE:CD2	1:D:133:LEU:CD2	3.01	0.43
1:C:137:ALA:CB	1:C:141:GLN:NE2	2.81	0.43
1:D:13:LEU:HA	1:D:13:LEU:HD12	1.69	0.43
1:B:26:THR:HG22	1:B:27:ILE:N	2.33	0.43
1:E:68:ASN:O	1:E:71:VAL:HB	2.18	0.43
1:A:86:PRO:HB2	1:A:122:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HD2	1:A:60:LYS:C	2.39	0.42
1:A:105:GLN:O	1:A:105:GLN:HG2	2.17	0.42
1:A:3:ILE:HD11	1:A:97:CYS:HA	1.99	0.42
1:D:52:ARG:NH2	1:D:62:GLU:OE1	2.51	0.42
1:C:1:MET:HG2	1:C:158:TRP:CD2	2.55	0.42
1:D:13:LEU:CD1	1:D:29:ILE:HG13	2.49	0.42
1:B:115:THR:HG22	1:B:119:ARG:HD2	2.00	0.42
1:A:94:VAL:O	1:A:97:CYS:HB2	2.20	0.42
1:E:141:GLN:HG2	1:E:141:GLN:H	1.51	0.42
1:C:39:LEU:HA	1:C:39:LEU:HD12	1.70	0.42
1:B:138:TRP:CA	1:B:141:GLN:HG3	2.50	0.42
1:B:138:TRP:HA	1:B:141:GLN:HG3	2.02	0.42
1:D:124:LYS:HG3	1:D:126:TRP:CZ2	2.54	0.42
1:E:1:MET:HB3	1:E:158:TRP:CD1	2.54	0.42
1:B:120:MET:CE	1:B:128:ALA:CB	2.97	0.42
1:A:122:GLN:C	1:A:124:LYS:H	2.22	0.42
1:E:91:LEU:HD23	1:E:91:LEU:HA	1.69	0.42
1:D:116:ASN:N	1:D:116:ASN:HD22	2.17	0.42
1:A:52:ARG:O	1:A:54:CYS:SG	2.77	0.42
1:E:46:LEU:O	1:E:49:ALA:HB3	2.20	0.42
1:B:24:TYR:CD1	1:B:35:LYS:HG2	2.55	0.42
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.86	0.42
1:A:46:LEU:O	1:A:50:ILE:HG12	2.20	0.41
1:E:9:ILE:HG21	1:E:9:ILE:HD13	1.76	0.41
1:D:114:PHE:HD2	1:D:133:LEU:HD23	1.82	0.41
1:B:146:ALA:O	1:B:150:ILE:HD12	2.20	0.41
1:A:142:THR:O	1:A:142:THR:OG1	2.36	0.41
1:C:8:ARG:O	1:C:12:GLY:N	2.53	0.41
1:B:1:MET:HG2	1:B:5:GLU:HB2	2.01	0.41
1:B:29:ILE:HG22	1:B:29:ILE:O	2.19	0.41
1:D:24:TYR:CE1	1:D:35:LYS:CG	3.03	0.41
1:C:75:VAL:CG1	1:C:79:LEU:CD1	2.98	0.41
1:E:51:GLY:O	1:E:52:ARG:HB3	2.20	0.41
1:D:84:LEU:CA	1:D:87:VAL:HG23	2.48	0.41
1:D:92:ASP:OD1	1:D:95:ARG:HG3	2.20	0.41
1:A:11:GLU:O	1:A:12:GLY:O	2.38	0.41
1:E:27:ILE:CD1	1:E:58:ILE:CD1	2.98	0.41
1:E:81:ASN:OD1	1:E:83:LYS:HB2	2.20	0.41
1:E:120:MET:HB3	1:E:125:ARG:HB2	2.01	0.41
1:D:26:THR:HA	1:D:31:HIS:O	2.20	0.41
1:D:20:ASP:OD1	1:D:22:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:GLU:O	1:A:111:VAL:HG23	2.21	0.41
1:C:120:MET:HB2	1:C:120:MET:HE2	1.79	0.41
1:D:99:LEU:HD12	1:D:99:LEU:O	2.21	0.41
1:D:39:LEU:O	1:D:42:ALA:HB3	2.21	0.41
1:A:102:MET:HE1	1:A:133:LEU:CD2	2.46	0.41
1:A:141:GLN:H	1:A:141:GLN:HG2	1.71	0.41
1:A:91:LEU:HD23	1:A:91:LEU:HA	1.73	0.41
1:E:90:SER:O	1:E:124:LYS:NZ	2.48	0.41
1:A:1:MET:HB3	1:A:158:TRP:NE1	2.35	0.41
1:D:84:LEU:HA	1:D:87:VAL:HG21	2.00	0.41
1:C:7:LEU:HD12	1:C:67:PHE:CE1	2.56	0.41
1:D:95:ARG:NE	1:D:153:PHE:O	2.35	0.41
1:E:99:LEU:O	1:E:99:LEU:HD23	2.21	0.41
1:C:39:LEU:HG	1:C:39:LEU:O	2.19	0.41
1:C:25:TYR:CE1	1:C:39:LEU:HD13	2.56	0.41
1:C:143:PRO:HD2	1:C:144:ASN:H	1.85	0.41
1:A:13:LEU:HD12	1:A:29:ILE:HG13	2.01	0.41
1:A:85:LYS:CB	1:A:86:PRO:CD	2.98	0.41
1:C:13:LEU:HA	1:C:13:LEU:HD12	1.86	0.41
1:C:2:ASN:H	1:C:5:GLU:HB2	1.85	0.41
1:C:24:TYR:CD2	1:C:35:LYS:HE2	2.56	0.41
1:D:139:TYR:O	1:D:143:PRO:HA	2.20	0.40
1:C:15:LEU:HB3	1:C:58:ILE:O	2.20	0.40
1:E:32:LEU:O	1:E:32:LEU:HD23	2.21	0.40
1:A:32:LEU:HD23	1:A:34:THR:H	1.86	0.40
1:D:1:MET:CE	1:D:5:GLU:HB3	2.52	0.40
1:D:26:THR:CG2	1:D:27:ILE:H	2.34	0.40
1:E:120:MET:HE1	1:E:128:ALA:O	2.22	0.40
1:C:60:LYS:HZ2	1:C:60:LYS:C	2.24	0.40
1:D:120:MET:HE3	1:D:129:ALA:HA	2.02	0.40
1:D:138:TRP:HA	1:D:141:GLN:HE21	1.87	0.40
1:E:85:LYS:CB	1:E:86:PRO:CD	3.00	0.40
1:B:157:THR:OG1	1:B:159:ASP:OD2	2.33	0.40
1:C:99:LEU:O	1:C:103:VAL:HG23	2.21	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	162/164 (99%)	135 (83%)	15 (9%)	12 (7%)	1 3
1	B	162/164 (99%)	137 (85%)	17 (10%)	8 (5%)	3 10
1	C	162/164 (99%)	139 (86%)	19 (12%)	4 (2%)	7 27
1	D	162/164 (99%)	134 (83%)	20 (12%)	8 (5%)	3 10
1	E	162/164 (99%)	136 (84%)	22 (14%)	4 (2%)	7 27
All	All	810/820 (99%)	681 (84%)	93 (12%)	36 (4%)	3 12

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	ARG
1	A	93	ALA
1	A	114	PHE
1	A	162	LYS
1	A	163	ASN
1	B	162	LYS
1	B	163	ASN
1	C	162	LYS
1	D	114	PHE
1	D	162	LYS
1	D	163	ASN
1	E	53	ASN
1	A	12	GLY
1	A	115	THR
1	C	115	THR
1	C	158	TRP
1	C	163	ASN
1	D	126	TRP
1	D	160	ALA
1	A	52	ARG
1	B	46	LEU

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Mol	Chain	Res	Type
1	B	47	ASP
1	B	80	ARG
1	B	115	THR
1	D	130	ALA
1	E	109	THR
1	A	53	ASN
1	A	85	LYS
1	A	123	GLN
1	A	138	TRP
1	E	158	TRP
1	D	93	ALA
1	E	52	ARG
1	B	107	GLY
1	B	29	ILE
1	D	143	PRO

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	132/132 (100%)	102 (77%)	30 (23%)	1 3
1	B	132/132 (100%)	112 (85%)	20 (15%)	3 10
1	C	132/132 (100%)	109 (83%)	23 (17%)	2 7
1	D	132/132 (100%)	105 (80%)	27 (20%)	1 4
1	E	132/132 (100%)	115 (87%)	17 (13%)	5 16
All	All	660/660 (100%)	543 (82%)	117 (18%)	2 7

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	8	ARG
1	A	16	LYS
1	A	36	SER

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Mol	Chain	Res	Type
1	A	40	ASN
1	A	52	ARG
1	A	54	CYS
1	A	60	LYS
1	A	65	LYS
1	A	83	LYS
1	A	85	LYS
1	A	90	SER
1	A	94	VAL
1	A	104	PHE
1	A	106	MET
1	A	109	THR
1	A	111	VAL
1	A	116	ASN
1	A	117	SER
1	A	119	ARG
1	A	122	GLN
1	A	123	GLN
1	A	125	ARG
1	A	127	ASP
1	A	141	GLN
1	A	147	LYS
1	A	151	THR
1	A	155	THR
1	A	157	THR
1	A	164	LEU
1	B	1	MET
1	B	21	THR
1	B	32	LEU
1	B	36	SER
1	B	38	SER
1	B	40	ASN
1	B	48	LYS
1	B	53	ASN
1	B	59	THR
1	B	60	LYS
1	B	65	LYS
1	B	104	PHE
1	B	116	ASN
1	B	117	SER
1	B	123	GLN
1	B	125	ARG

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Mol	Chain	Res	Type
1	B	127	ASP
1	B	154	ARG
1	B	157	THR
1	B	164	LEU
1	C	1	MET
1	C	27	ILE
1	C	32	LEU
1	C	43	LYS
1	C	48	LYS
1	C	50	ILE
1	C	53	ASN
1	C	60	LYS
1	C	65	LYS
1	C	84	LEU
1	C	90	SER
1	C	96	ARG
1	C	104	PHE
1	C	116	ASN
1	C	117	SER
1	C	120	MET
1	C	122	GLN
1	C	141	GLN
1	C	151	THR
1	C	152	THR
1	C	154	ARG
1	C	155	THR
1	C	164	LEU
1	D	1	MET
1	D	10	ASP
1	D	32	LEU
1	D	35	LYS
1	D	38	SER
1	D	40	ASN
1	D	48	LYS
1	D	52	ARG
1	D	53	ASN
1	D	72	ASP
1	D	84	LEU
1	D	87	VAL
1	D	89	ASP
1	D	90	SER
1	D	92	ASP

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Mol	Chain	Res	Type
1	D	95	ARG
1	D	101	ASN
1	D	104	PHE
1	D	106	MET
1	D	109	THR
1	D	119	ARG
1	D	127	ASP
1	D	141	GLN
1	D	151	THR
1	D	154	ARG
1	D	159	ASP
1	D	164	LEU
1	E	2	ASN
1	E	6	MET
1	E	44	SER
1	E	46	LEU
1	E	50	ILE
1	E	53	ASN
1	E	59	THR
1	E	76	ARG
1	E	83	LYS
1	E	90	SER
1	E	99	LEU
1	E	104	PHE
1	E	119	ARG
1	E	122	GLN
1	E	125	ARG
1	E	141	GLN
1	E	157	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	55	ASN
1	A	116	ASN
1	A	122	GLN
1	A	141	GLN
1	B	68	ASN
1	B	69	GLN
1	B	122	GLN
1	B	123	GLN

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Mol	Chain	Res	Type
1	B	141	GLN
1	B	144	ASN
1	C	2	ASN
1	C	53	ASN
1	C	69	GLN
1	C	141	GLN
1	D	116	ASN
1	D	122	GLN
1	D	141	GLN
1	E	31	HIS
1	E	53	ASN
1	E	68	ASN
1	E	116	ASN
1	E	122	GLN
1	E	140	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	160/164 (97%)	-0.58	2 (1%) 79 78	17, 40, 65, 82	0
1	B	160/164 (97%)	-0.87	0 100 100	2, 25, 51, 67	0
1	C	160/164 (97%)	-0.99	0 100 100	3, 18, 42, 64	0
1	D	160/164 (97%)	-0.72	0 100 100	5, 28, 63, 73	0
1	E	160/164 (97%)	-0.72	0 100 100	8, 31, 58, 71	0
All	All	800/820 (97%)	-0.77	2 (0%) 94 94	2, 29, 59, 82	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ASN	3.4
1	A	119	ARG	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.