



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:51 am GMT

PDB ID : 1AKM
Title : ORNITHINE TRANSCARBAMYLASE FROM ESCHERICHIA COLI
Authors : Head, J.F.; Seaton, B.; Jin, L.
Deposited on : 1997-05-23
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

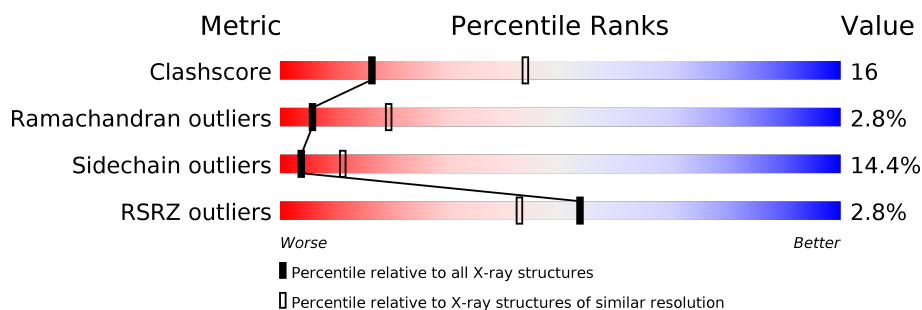
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	333	<div> <div>4%</div> <div>51% 34% 9% . .</div> </div>
1	B	333	<div> <div>2%</div> <div>60% 29% 5% . .</div> </div>
1	C	333	<div> <div>3%</div> <div>59% 29% 7% . .</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7482 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.

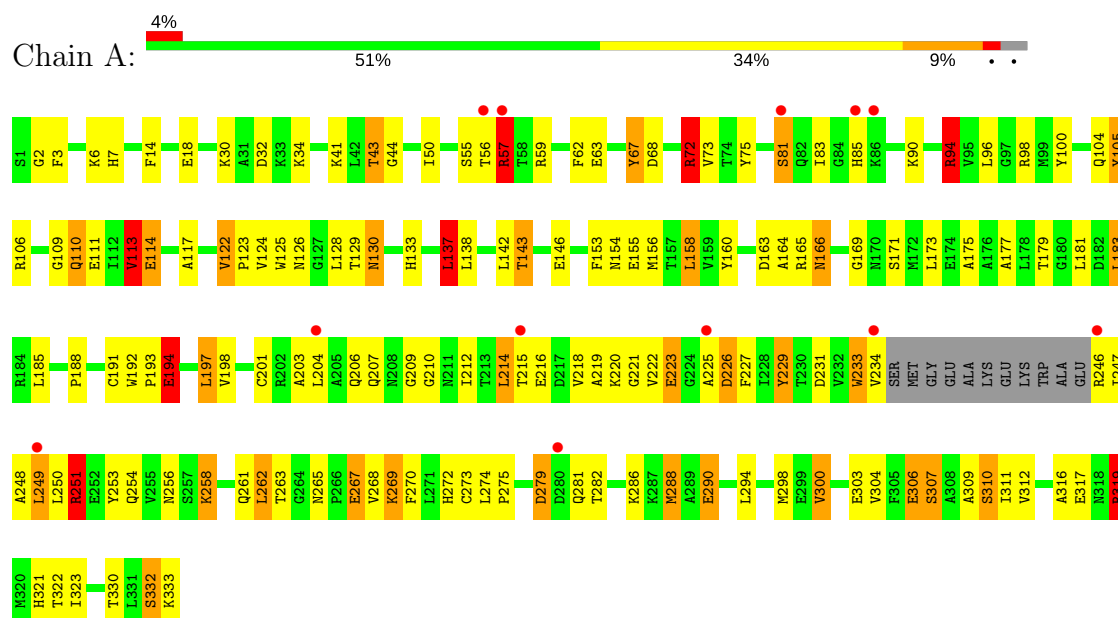
- Molecule 1 is a protein called ORNITHINE TRANSCARBAMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			
1	B	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			
1	C	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			

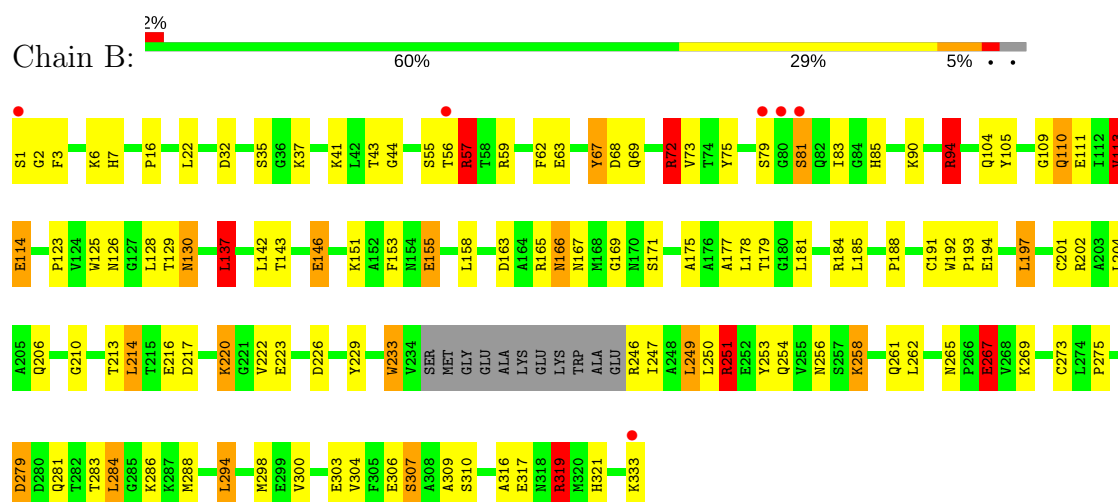
3 Residue-property plots

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: ORNITHINE TRANSCARBAMYLASE

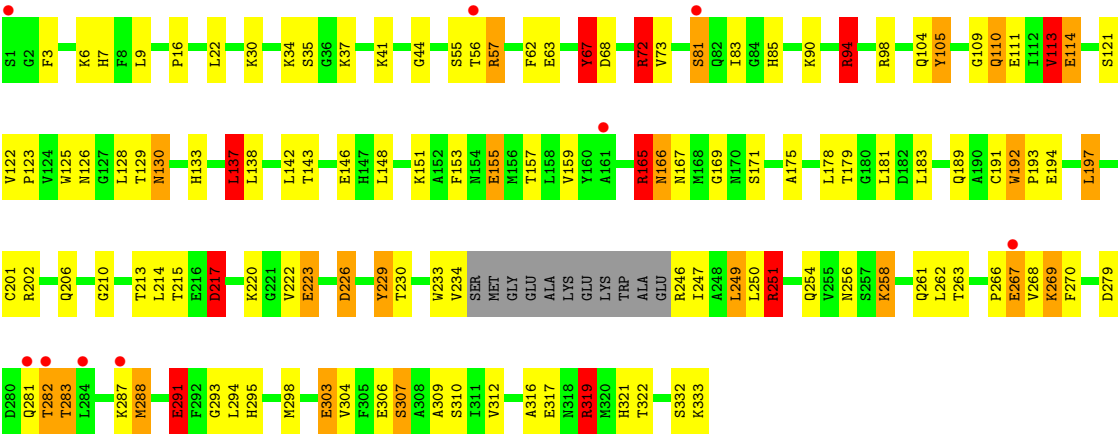


• Molecule 1: ORNITHINE TRANSCARBAMYLASE



• Molecule 1: ORNITHINE TRANSCARBAMYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	104.60Å 104.60Å 86.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80 34.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (6.00-2.80) 95.7 (34.24-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.229 , 0.302 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.032 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7482	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	3/2539 (0.1%)	1.64	32/3430 (0.9%)
1	B	1.00	4/2539 (0.2%)	1.66	36/3430 (1.0%)
1	C	0.98	2/2539 (0.1%)	1.63	36/3430 (1.0%)
All	All	0.99	9/7617 (0.1%)	1.64	104/10290 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	TRP	CG-CD2	-7.07	1.31	1.43
1	B	125	TRP	CG-CD2	-6.52	1.32	1.43
1	B	57	ARG	NE-CZ	5.74	1.40	1.33
1	A	57	ARG	NE-CZ	5.61	1.40	1.33
1	A	125	TRP	CG-CD2	-5.40	1.34	1.43
1	B	125	TRP	CD1-NE1	-5.24	1.29	1.38
1	C	125	TRP	NE1-CE2	-5.12	1.30	1.37
1	B	192	TRP	CD1-NE1	-5.09	1.29	1.38
1	A	165	ARG	NE-CZ	5.04	1.39	1.33

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH1	20.03	130.32	120.30
1	A	57	ARG	NE-CZ-NH1	18.07	129.34	120.30
1	B	57	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	57	ARG	NE-CZ-NH2	-15.60	112.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	B	94	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	B	94	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	156	MET	CG-SD-CE	-9.15	85.55	100.20
1	A	72	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	233	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	C	94	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	C	233	TRP	CD1-CG-CD2	8.89	113.41	106.30
1	A	67	TYR	CB-CG-CD2	-8.73	115.76	121.00
1	C	94	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	114	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	A	288	MET	CG-SD-CE	-8.25	87.00	100.20
1	C	319	ARG	NE-CZ-NH1	7.89	124.24	120.30
1	C	233	TRP	CE2-CD2-CG	-7.76	101.09	107.30
1	A	94	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	72	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	59	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	125	TRP	CE2-CD2-CG	-7.32	101.44	107.30
1	C	251	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	C	202	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	233	TRP	CD1-CG-CD2	7.19	112.06	106.30
1	A	233	TRP	CE2-CD2-CG	-7.06	101.65	107.30
1	B	192	TRP	CD1-CG-CD2	7.06	111.95	106.30
1	B	192	TRP	CE2-CD2-CG	-6.99	101.71	107.30
1	C	72	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	114	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	A	192	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	B	202	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	194	GLU	CA-C-N	-6.86	102.11	117.20
1	B	251	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	C	137	LEU	CA-CB-CG	-6.82	99.62	115.30
1	B	233	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	B	273	CYS	CA-C-N	6.54	131.59	117.20
1	C	192	TRP	CE2-CD2-CG	-6.48	102.12	107.30
1	C	67	TYR	CB-CG-CD2	-6.46	117.12	121.00
1	C	113	VAL	CB-CA-C	-6.39	99.26	111.40
1	B	67	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	B	113	VAL	CB-CA-C	-6.37	99.30	111.40
1	B	114	GLU	OE1-CD-OE2	-6.36	115.67	123.30
1	C	125	TRP	CE2-CD2-CG	-6.32	102.25	107.30
1	C	319	ARG	CB-CG-CD	-6.31	95.19	111.60
1	C	269	LYS	CG-CD-CE	6.28	130.75	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	32	ASP	CB-CG-OD1	6.17	123.86	118.30
1	B	137	LEU	CA-CB-CG	-6.15	101.16	115.30
1	C	319	ARG	CD-NE-CZ	-6.09	115.07	123.60
1	C	192	TRP	CD1-CG-CD2	6.06	111.15	106.30
1	A	122	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	A	229	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	75	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	113	VAL	CB-CA-C	-5.85	100.28	111.40
1	C	268	VAL	CG1-CB-CG2	-5.82	101.58	110.90
1	A	137	LEU	CA-CB-CG	-5.80	101.95	115.30
1	C	229	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	319	ARG	CB-CG-CD	-5.67	96.84	111.60
1	B	59	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	214	LEU	CA-CB-CG	5.65	128.29	115.30
1	B	269	LYS	CG-CD-CE	5.65	128.85	111.90
1	B	267	GLU	CA-CB-CG	5.64	125.82	113.40
1	A	68	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	184	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	125	TRP	CE2-CD2-CG	-5.58	102.83	107.30
1	C	267	GLU	CA-CB-CG	5.57	125.65	113.40
1	A	192	TRP	CD1-CG-CD2	5.57	110.75	106.30
1	C	68	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	216	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	B	294	LEU	CA-CB-CG	5.52	128.00	115.30
1	B	273	CYS	O-C-N	-5.51	113.88	122.70
1	C	122	VAL	CA-CB-CG1	-5.47	102.69	110.90
1	B	222	VAL	CG1-CB-CG2	-5.45	102.17	110.90
1	C	165	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	68	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	319	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	B	146	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	A	251	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	57	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
1	A	300	VAL	CB-CA-C	-5.35	101.24	111.40
1	A	105	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	B	125	TRP	NE1-CE2-CD2	5.30	112.61	107.30
1	A	194	GLU	O-C-N	5.29	131.17	122.70
1	C	191	CYS	N-CA-CB	-5.28	101.09	110.60
1	C	125	TRP	NE1-CE2-CD2	5.27	112.57	107.30
1	B	216	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	32	ASP	CB-CG-OD1	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	319	ARG	CB-CG-CD	-5.24	97.97	111.60
1	A	160	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	B	75	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	B	57	ARG	CB-CA-C	-5.20	100.00	110.40
1	C	303	GLU	CA-CB-CG	5.20	124.84	113.40
1	B	267	GLU	O-C-N	-5.18	114.41	122.70
1	C	282	THR	CA-CB-CG2	-5.17	105.17	112.40
1	A	233	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	C	57	ARG	CB-CG-CD	-5.14	98.24	111.60
1	C	105	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	165	ARG	CA-CB-CG	5.12	124.66	113.40
1	B	125	TRP	CD1-CG-CD2	5.10	110.38	106.30
1	A	332	SER	N-CA-CB	-5.09	102.87	110.50
1	B	319	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	217	ASP	CB-CA-C	-5.04	100.31	110.40
1	C	125	TRP	CD1-CG-CD2	5.03	110.33	106.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	67	TYR	Sidechain

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	2494	0	2474	103	0
1	B	2494	0	2474	68	0
1	C	2494	0	2474	74	0
All	All	7482	0	7422	239	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 16.

All (239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD22	1:C:201:CYS:SG	2.21	0.80
1:A:72:ARG:HD3	1:C:67:TYR:HB3	1.62	0.79
1:A:137:LEU:HD13	1:A:171:SER:HB3	1.66	0.77
1:B:137:LEU:HD13	1:B:171:SER:HB3	1.67	0.76
1:C:7:HIS:HD2	1:C:123:PRO:HA	1.50	0.75
1:C:137:LEU:HD13	1:C:171:SER:HB3	1.67	0.75
1:A:304:VAL:O	1:A:307:SER:HB2	1.88	0.73
1:B:304:VAL:O	1:B:307:SER:HB2	1.89	0.73
1:A:3:PHE:HA	1:A:6:LYS:HE2	1.70	0.72
1:B:197:LEU:HD22	1:B:201:CYS:SG	2.29	0.71
1:A:197:LEU:HD22	1:A:201:CYS:SG	2.31	0.71
1:A:109:GLY:HA2	1:A:130:ASN:ND2	2.06	0.70
1:C:304:VAL:O	1:C:307:SER:HB2	1.92	0.69
1:A:206:GLN:HA	1:A:210:GLY:O	1.92	0.69
1:A:90:LYS:O	1:A:94:ARG:HD3	1.95	0.67
1:C:166:ASN:ND2	1:C:169:GLY:H	1.92	0.67
1:B:7:HIS:HD2	1:B:123:PRO:HA	1.57	0.67
1:C:206:GLN:HA	1:C:210:GLY:O	1.95	0.66
1:C:7:HIS:CD2	1:C:123:PRO:HA	2.31	0.66
1:C:90:LYS:O	1:C:94:ARG:HD3	1.97	0.65
1:A:215:THR:HG21	1:A:221:GLY:HA3	1.77	0.65
1:B:126:ASN:HD21	1:B:129:THR:HG23	1.62	0.65
1:B:3:PHE:HA	1:B:6:LYS:HE2	1.79	0.65
1:A:62:PHE:CZ	1:A:104:GLN:HG3	2.32	0.64
1:B:206:GLN:HA	1:B:210:GLY:O	1.97	0.64
1:B:62:PHE:CZ	1:B:104:GLN:HG3	2.33	0.64
1:B:44:GLY:HA2	1:B:72:ARG:NH2	2.14	0.63
1:A:44:GLY:HA2	1:A:72:ARG:NH2	2.14	0.63
1:C:44:GLY:HA2	1:C:72:ARG:NH2	2.14	0.63
1:B:90:LYS:O	1:B:94:ARG:HD3	1.99	0.62
1:C:63:GLU:HG2	1:C:73:VAL:HG11	1.82	0.62
1:C:189:GLN:HA	1:C:192:TRP:CE2	2.34	0.62
1:A:6:LYS:HE3	1:A:14:PHE:HE1	1.65	0.62
1:C:3:PHE:HA	1:C:6:LYS:HE2	1.82	0.62
1:A:163:ASP:HA	1:A:191:CYS:HB3	1.82	0.62
1:C:126:ASN:HD21	1:C:129:THR:HG23	1.65	0.61
1:B:63:GLU:HG2	1:B:73:VAL:HG11	1.82	0.61
1:A:166:ASN:ND2	1:A:169:GLY:H	1.99	0.61
1:C:109:GLY:HA2	1:C:130:ASN:ND2	2.16	0.61
1:A:153:PHE:HB3	1:A:179:THR:HG23	1.83	0.61
1:C:126:ASN:ND2	1:C:129:THR:HG23	2.16	0.61
1:C:307:SER:HB3	1:C:309:ALA:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:OD1	1:A:267:GLU:HG3	2.02	0.60
1:A:63:GLU:HG2	1:A:73:VAL:HG11	1.83	0.60
1:A:3:PHE:CZ	1:A:18:GLU:HB3	2.37	0.60
1:A:100:TYR:O	1:A:122:VAL:HG11	2.02	0.60
1:A:137:LEU:HD22	1:A:175:ALA:HB2	1.83	0.60
1:A:270:PHE:HD2	1:A:310:SER:HB3	1.67	0.60
1:A:226:ASP:O	1:A:269:LYS:HD2	2.01	0.59
1:C:288:MET:N	1:C:288:MET:SD	2.75	0.59
1:B:166:ASN:ND2	1:B:169:GLY:H	2.01	0.59
1:C:153:PHE:HB3	1:C:179:THR:HG23	1.84	0.59
1:B:185:LEU:HB2	1:B:214:LEU:HD13	1.84	0.59
1:A:164:ALA:O	1:A:169:GLY:HA3	2.02	0.58
1:A:263:THR:HG21	1:A:268:VAL:HG21	1.85	0.58
1:B:126:ASN:ND2	1:B:129:THR:HG23	2.18	0.58
1:C:81:SER:OG	1:C:85:HIS:HB3	2.04	0.57
1:A:225:ALA:HB3	1:A:263:THR:HG22	1.86	0.57
1:B:188:PRO:HD3	1:B:253:TYR:CE2	2.39	0.57
1:C:142:LEU:O	1:C:146:GLU:HG3	2.04	0.57
1:B:67:TYR:HB3	1:C:72:ARG:HD3	1.87	0.57
1:C:3:PHE:CZ	1:C:22:LEU:HG	2.39	0.57
1:C:279:ASP:HB3	1:C:281:GLN:H	1.70	0.57
1:A:7:HIS:HD2	1:A:124:VAL:H	1.50	0.57
1:C:3:PHE:HA	1:C:6:LYS:CE	2.35	0.57
1:B:109:GLY:HA2	1:B:130:ASN:ND2	2.20	0.56
1:B:284:LEU:O	1:B:288:MET:HG2	2.05	0.56
1:B:35:SER:OG	1:B:37:LYS:NZ	2.39	0.56
1:B:113:VAL:HG22	1:B:129:THR:HG21	1.87	0.56
1:A:142:LEU:O	1:A:146:GLU:HG3	2.05	0.56
1:A:307:SER:HB3	1:A:309:ALA:H	1.68	0.56
1:A:44:GLY:HA2	1:A:72:ARG:HH22	1.70	0.56
1:A:273:CYS:O	1:A:273:CYS:SG	2.63	0.56
1:C:62:PHE:CZ	1:C:104:GLN:HG3	2.41	0.56
1:B:188:PRO:HG2	1:B:191:CYS:SG	2.46	0.55
1:C:293:GLY:HA2	1:C:295:HIS:CE1	2.41	0.55
1:C:44:GLY:HA2	1:C:72:ARG:HH22	1.72	0.55
1:A:113:VAL:HG22	1:A:129:THR:HG21	1.88	0.55
1:B:137:LEU:HD22	1:B:175:ALA:HB2	1.88	0.55
1:B:294:LEU:HD13	1:B:298:MET:HG2	1.89	0.55
1:B:217:ASP:CG	1:B:220:LYS:HB3	2.28	0.54
1:B:254:GLN:HG3	1:B:298:MET:O	2.08	0.54
1:B:7:HIS:CD2	1:B:123:PRO:HA	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:CZ	1:B:22:LEU:HG	2.43	0.54
1:B:265:ASN:OD1	1:B:267:GLU:HG3	2.07	0.53
1:B:153:PHE:HB3	1:B:179:THR:HG23	1.89	0.53
1:C:137:LEU:HD22	1:C:175:ALA:HB2	1.89	0.53
1:C:113:VAL:HG22	1:C:129:THR:HG21	1.90	0.53
1:C:230:THR:HG22	1:C:270:PHE:HE1	1.74	0.53
1:A:188:PRO:HG3	1:A:249:LEU:HD22	1.91	0.53
1:A:7:HIS:CE1	1:A:117:ALA:HB1	2.44	0.53
1:A:212:ILE:HG22	1:A:214:LEU:CD2	2.38	0.53
1:B:105:TYR:CD2	1:B:113:VAL:HG13	2.43	0.53
1:A:105:TYR:CD2	1:A:113:VAL:HG13	2.44	0.52
1:A:126:ASN:ND2	1:A:129:THR:HG23	2.24	0.52
1:A:67:TYR:HB3	1:B:72:ARG:HD3	1.92	0.52
1:C:105:TYR:CD2	1:C:113:VAL:HG13	2.45	0.52
1:A:215:THR:HG21	1:A:221:GLY:CA	2.40	0.51
1:B:153:PHE:CB	1:B:179:THR:HG23	2.40	0.51
1:A:219:ALA:HB2	1:A:262:LEU:HD22	1.92	0.51
1:A:153:PHE:HB3	1:A:179:THR:CG2	2.40	0.51
1:C:3:PHE:CE2	1:C:22:LEU:HG	2.46	0.51
1:B:217:ASP:HB3	1:B:220:LYS:HB3	1.93	0.51
1:A:227:PHE:HA	1:A:269:LYS:O	2.11	0.51
1:A:126:ASN:HD21	1:A:129:THR:HG23	1.76	0.50
1:A:188:PRO:HG2	1:A:191:CYS:SG	2.52	0.50
1:B:179:THR:CG2	1:B:181:LEU:HG	2.42	0.50
1:A:279:ASP:HB3	1:A:281:GLN:H	1.75	0.50
1:B:62:PHE:CE2	1:B:104:GLN:HG3	2.47	0.50
1:B:81:SER:OG	1:B:85:HIS:HB3	2.11	0.50
1:C:165:ARG:HB2	1:C:192:TRP:O	2.12	0.50
1:A:173:LEU:HD11	1:A:193:PRO:HB2	1.94	0.50
1:B:166:ASN:HD22	1:B:169:GLY:H	1.59	0.49
1:A:212:ILE:HG22	1:A:214:LEU:HD21	1.95	0.49
1:B:316:ALA:O	1:B:319:ARG:HB2	2.11	0.49
1:A:256:ASN:OD1	1:A:258:LYS:HB3	2.12	0.49
1:B:110:GLN:O	1:B:113:VAL:HG23	2.13	0.49
1:A:194:GLU:OE1	1:A:197:LEU:HB2	2.13	0.49
1:A:179:THR:CG2	1:A:181:LEU:HG	2.43	0.49
1:B:249:LEU:HD13	1:B:250:LEU:HG	1.94	0.49
1:C:153:PHE:HB3	1:C:179:THR:CG2	2.42	0.49
1:C:16:PRO:HB3	1:C:178:LEU:O	2.12	0.49
1:A:81:SER:OG	1:A:85:HIS:HB3	2.14	0.48
1:A:281:GLN:O	1:A:286:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:PHE:CB	1:A:179:THR:HG23	2.43	0.48
1:B:307:SER:HB3	1:B:309:ALA:H	1.78	0.48
1:C:247:ILE:HG23	1:C:294:LEU:HD11	1.95	0.48
1:A:317:GLU:OE2	1:A:321:HIS:HE1	1.96	0.48
1:B:317:GLU:OE2	1:B:321:HIS:HE1	1.97	0.48
1:C:179:THR:CG2	1:C:181:LEU:HG	2.44	0.48
1:C:234:VAL:HG12	1:C:246:ARG:HB3	1.96	0.48
1:A:188:PRO:CG	1:A:249:LEU:HD22	2.43	0.48
1:C:317:GLU:OE2	1:C:321:HIS:HE1	1.97	0.48
1:B:41:LYS:NZ	1:B:333:LYS:O	2.47	0.47
1:C:9:LEU:HD22	1:C:113:VAL:HB	1.96	0.47
1:A:62:PHE:CE2	1:A:104:GLN:HG3	2.49	0.47
1:C:30:LYS:O	1:C:34:LYS:HG3	2.14	0.47
1:A:231:ASP:HA	1:A:272:HIS:CE1	2.49	0.47
1:C:151:LYS:NZ	1:C:155:GLU:HB2	2.30	0.47
1:C:153:PHE:CB	1:C:179:THR:HG23	2.44	0.47
1:C:222:VAL:HG13	1:C:263:THR:HG22	1.97	0.47
1:A:133:HIS:CE1	1:A:319:ARG:NH2	2.83	0.47
1:B:142:LEU:O	1:B:146:GLU:HG3	2.15	0.47
1:B:16:PRO:HB3	1:B:178:LEU:O	2.15	0.47
1:A:3:PHE:HZ	1:A:18:GLU:HB3	1.80	0.47
1:A:254:GLN:HG3	1:A:298:MET:O	2.15	0.46
1:A:6:LYS:O	1:A:123:PRO:HB3	2.15	0.46
1:B:44:GLY:HA2	1:B:72:ARG:HH22	1.78	0.46
1:A:185:LEU:HB2	1:A:214:LEU:HD13	1.96	0.46
1:B:153:PHE:HB3	1:B:179:THR:CG2	2.45	0.46
1:A:3:PHE:HE1	1:A:14:PHE:CD1	2.33	0.46
1:B:279:ASP:HB3	1:B:281:GLN:H	1.80	0.46
1:C:249:LEU:HD12	1:C:249:LEU:H	1.80	0.46
1:A:188:PRO:HD3	1:A:253:TYR:CE2	2.51	0.46
1:C:110:GLN:O	1:C:113:VAL:HG23	2.16	0.46
1:C:217:ASP:HB2	1:C:220:LYS:HB3	1.98	0.46
1:C:41:LYS:NZ	1:C:333:LYS:O	2.49	0.46
1:A:137:LEU:CD1	1:A:171:SER:HB3	2.40	0.46
1:A:234:VAL:HG21	1:A:288:MET:CE	2.46	0.46
1:B:151:LYS:NZ	1:B:155:GLU:HB2	2.30	0.46
1:C:175:ALA:O	1:C:179:THR:HB	2.16	0.46
1:C:256:ASN:OD1	1:C:258:LYS:HB3	2.15	0.46
1:C:159:VAL:HG21	1:C:222:VAL:HA	1.98	0.45
1:C:223:GLU:O	1:C:263:THR:HA	2.16	0.45
1:A:233:TRP:O	1:A:246:ARG:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:HB1	1:B:204:LEU:HD22	1.99	0.45
1:A:6:LYS:HE3	1:A:14:PHE:CE1	2.50	0.45
1:B:193:PRO:HD2	1:B:214:LEU:HD11	1.97	0.45
1:A:7:HIS:HD2	1:A:123:PRO:HA	1.81	0.45
1:B:286:LYS:HE3	1:B:286:LYS:HB2	1.66	0.45
1:C:130:ASN:O	1:C:167:ASN:HB3	2.17	0.45
1:B:217:ASP:CB	1:B:220:LYS:HB3	2.47	0.45
1:B:57:ARG:NH2	1:B:275:PRO:HG3	2.32	0.45
1:C:62:PHE:CE2	1:C:104:GLN:HG3	2.52	0.45
1:A:30:LYS:O	1:A:34:LYS:HG3	2.17	0.45
1:B:163:ASP:HA	1:B:191:CYS:HB3	1.98	0.45
1:A:98:ARG:NH1	1:C:317:GLU:OE1	2.50	0.45
1:B:113:VAL:CG2	1:B:129:THR:HG21	2.47	0.44
1:B:151:LYS:HZ2	1:B:155:GLU:HB2	1.81	0.44
1:C:287:LYS:O	1:C:291:GLU:HB2	2.17	0.44
1:A:247:ILE:O	1:A:251:ARG:HB2	2.16	0.44
1:C:35:SER:OG	1:C:37:LYS:NZ	2.48	0.44
1:A:113:VAL:CG2	1:A:129:THR:HG21	2.47	0.44
1:B:105:TYR:HD2	1:B:113:VAL:HG13	1.82	0.44
1:B:249:LEU:HD12	1:B:249:LEU:H	1.82	0.44
1:A:3:PHE:O	1:A:330:THR:HG22	2.17	0.44
1:A:194:GLU:O	1:A:198:VAL:HG23	2.18	0.44
1:C:316:ALA:O	1:C:319:ARG:HB2	2.18	0.44
1:A:179:THR:HG22	1:A:181:LEU:HG	1.99	0.44
1:A:225:ALA:HB3	1:A:263:THR:CG2	2.46	0.44
1:A:316:ALA:O	1:A:319:ARG:HB2	2.17	0.44
1:C:148:LEU:HD21	1:C:269:LYS:HZ1	1.82	0.43
1:A:177:ALA:HB1	1:A:204:LEU:HD22	2.01	0.43
1:A:7:HIS:CD2	1:A:123:PRO:HA	2.53	0.43
1:C:138:LEU:HB3	1:C:322:THR:HB	2.00	0.43
1:C:133:HIS:HE1	1:C:319:ARG:HH22	1.66	0.43
1:C:249:LEU:HD13	1:C:250:LEU:HG	2.00	0.43
1:B:2:GLY:O	1:B:6:LYS:HE2	2.19	0.43
1:A:110:GLN:O	1:A:113:VAL:HG23	2.18	0.43
1:A:219:ALA:CB	1:A:262:LEU:HD22	2.49	0.43
1:C:113:VAL:CG2	1:C:129:THR:HG21	2.47	0.43
1:C:291:GLU:CD	1:C:291:GLU:H	2.22	0.43
1:A:203:ALA:O	1:A:207:GLN:HB2	2.18	0.43
1:A:222:VAL:HG13	1:A:263:THR:HG22	2.01	0.43
1:C:151:LYS:HZ2	1:C:155:GLU:HB2	1.84	0.43
1:C:254:GLN:HG3	1:C:298:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:H	1:B:69:GLN:NE2	2.17	0.42
1:A:249:LEU:HD13	1:A:250:LEU:HG	2.00	0.42
1:A:98:ARG:HH11	1:A:98:ARG:HD2	1.71	0.42
1:B:130:ASN:O	1:B:167:ASN:HB3	2.19	0.42
1:B:233:TRP:O	1:B:246:ARG:HD2	2.19	0.42
1:A:7:HIS:CD2	1:A:124:VAL:H	2.35	0.42
1:A:220:LYS:O	1:A:223:GLU:HB2	2.20	0.42
1:B:179:THR:HG22	1:B:181:LEU:HG	2.01	0.42
1:C:193:PRO:HD2	1:C:214:LEU:HD11	2.00	0.42
1:A:143:THR:HG22	1:A:311:ILE:HD12	2.01	0.42
1:B:247:ILE:O	1:B:251:ARG:HB2	2.19	0.42
1:C:230:THR:HG22	1:C:270:PHE:CE1	2.54	0.41
1:A:306:GLU:OE1	1:B:94:ARG:NH2	2.51	0.41
1:A:41:LYS:NZ	1:A:333:LYS:O	2.53	0.41
1:A:233:TRP:CE3	1:A:247:ILE:HG12	2.56	0.41
1:B:256:ASN:OD1	1:B:258:LYS:HB3	2.21	0.41
1:A:105:TYR:HD2	1:A:113:VAL:HG13	1.84	0.41
1:A:154:ASN:OD1	1:A:209:GLY:HA3	2.21	0.41
1:A:158:LEU:HB3	1:A:183:LEU:HD23	2.01	0.41
1:C:247:ILE:O	1:C:251:ARG:HB2	2.21	0.41
1:A:290:GLU:HA	1:A:290:GLU:OE1	2.21	0.41
1:A:133:HIS:HE1	1:A:319:ARG:NH2	2.18	0.41
1:C:319:ARG:HH11	1:C:319:ARG:HD2	1.61	0.41
1:C:133:HIS:CE1	1:C:319:ARG:NH2	2.90	0.40
1:A:106:ARG:HH11	1:A:106:ARG:HD2	1.74	0.40
1:A:219:ALA:O	1:A:223:GLU:N	2.53	0.40
1:A:274:LEU:HD11	1:A:312:VAL:HG13	2.04	0.40
1:A:43:THR:O	1:A:43:THR:HG22	2.21	0.40
1:A:138:LEU:HB3	1:A:322:THR:HB	2.02	0.40
1:A:50:ILE:HD11	1:A:96:LEU:HD11	2.02	0.40
1:C:157:THR:H	1:C:226:ASP:HB2	1.85	0.40
1:B:317:GLU:OE1	1:C:98:ARG:NH1	2.55	0.40
1:A:57:ARG:NH2	1:A:275:PRO:HG3	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/333 (96%)	282 (89%)	24 (8%)	12 (4%)	4	12
1	B	318/333 (96%)	289 (91%)	22 (7%)	7 (2%)	8	26
1	C	318/333 (96%)	287 (90%)	23 (7%)	8 (2%)	6	22
All	All	954/999 (96%)	858 (90%)	69 (7%)	27 (3%)	6	19

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	223	GLU
1	B	128	LEU
1	B	223	GLU
1	C	128	LEU
1	C	223	GLU
1	C	291	GLU
1	A	294	LEU
1	A	2	GLY
1	A	218	VAL
1	A	282	THR
1	C	83	ILE
1	C	262	LEU
1	C	282	THR
1	C	283	THR
1	A	248	ALA
1	A	262	LEU
1	B	55	SER
1	C	55	SER
1	A	290	GLU
1	B	43	THR
1	B	79	SER
1	B	262	LEU
1	A	43	THR

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Mol	Chain	Res	Type
1	A	55	SER
1	A	83	ILE
1	B	83	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	262/270 (97%)	226 (86%)	36 (14%)	4	13
1	B	262/270 (97%)	225 (86%)	37 (14%)	4	12
1	C	262/270 (97%)	222 (85%)	40 (15%)	3	9
All	All	786/810 (97%)	673 (86%)	113 (14%)	4	11

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	57	ARG
1	A	72	ARG
1	A	81	SER
1	A	94	ARG
1	A	110	GLN
1	A	111	GLU
1	A	113	VAL
1	A	114	GLU
1	A	130	ASN
1	A	137	LEU
1	A	143	THR
1	A	155	GLU
1	A	158	LEU
1	A	166	ASN
1	A	183	LEU
1	A	194	GLU
1	A	197	LEU
1	A	214	LEU

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Mol	Chain	Res	Type
1	A	226	ASP
1	A	229	TYR
1	A	249	LEU
1	A	251	ARG
1	A	258	LYS
1	A	261	GLN
1	A	267	GLU
1	A	269	LYS
1	A	279	ASP
1	A	300	VAL
1	A	303	GLU
1	A	306	GLU
1	A	307	SER
1	A	310	SER
1	A	319	ARG
1	A	323	ILE
1	A	332	SER
1	B	1	SER
1	B	56	THR
1	B	57	ARG
1	B	72	ARG
1	B	81	SER
1	B	94	ARG
1	B	110	GLN
1	B	111	GLU
1	B	113	VAL
1	B	114	GLU
1	B	130	ASN
1	B	137	LEU
1	B	143	THR
1	B	155	GLU
1	B	158	LEU
1	B	165	ARG
1	B	166	ASN
1	B	194	GLU
1	B	197	LEU
1	B	213	THR
1	B	220	LYS
1	B	226	ASP
1	B	229	TYR
1	B	249	LEU
1	B	251	ARG

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Mol	Chain	Res	Type
1	B	258	LYS
1	B	261	GLN
1	B	267	GLU
1	B	279	ASP
1	B	283	THR
1	B	284	LEU
1	B	300	VAL
1	B	303	GLU
1	B	306	GLU
1	B	307	SER
1	B	310	SER
1	B	319	ARG
1	C	56	THR
1	C	57	ARG
1	C	72	ARG
1	C	81	SER
1	C	94	ARG
1	C	110	GLN
1	C	111	GLU
1	C	113	VAL
1	C	114	GLU
1	C	121	SER
1	C	130	ASN
1	C	137	LEU
1	C	143	THR
1	C	155	GLU
1	C	165	ARG
1	C	166	ASN
1	C	183	LEU
1	C	194	GLU
1	C	197	LEU
1	C	213	THR
1	C	215	THR
1	C	217	ASP
1	C	226	ASP
1	C	229	TYR
1	C	249	LEU
1	C	251	ARG
1	C	258	LYS
1	C	261	GLN
1	C	266	PRO
1	C	267	GLU

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Mol	Chain	Res	Type
1	C	283	THR
1	C	288	MET
1	C	291	GLU
1	C	303	GLU
1	C	306	GLU
1	C	307	SER
1	C	310	SER
1	C	312	VAL
1	C	319	ARG
1	C	332	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	69	GLN
1	A	85	HIS
1	A	110	GLN
1	A	126	ASN
1	A	130	ASN
1	A	133	HIS
1	A	166	ASN
1	A	295	HIS
1	A	321	HIS
1	B	7	HIS
1	B	69	GLN
1	B	85	HIS
1	B	110	GLN
1	B	126	ASN
1	B	130	ASN
1	B	133	HIS
1	B	166	ASN
1	B	206	GLN
1	B	321	HIS
1	C	7	HIS
1	C	69	GLN
1	C	85	HIS
1	C	126	ASN
1	C	130	ASN
1	C	133	HIS
1	C	166	ASN
1	C	321	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/333 (96%)	0.17	12 (3%) 42 31	2, 36, 67, 106	0
1	B	322/333 (96%)	-0.29	6 (1%) 67 58	2, 19, 47, 81	0
1	C	322/333 (96%)	-0.09	9 (2%) 53 43	3, 27, 58, 93	0
All	All	966/999 (96%)	-0.07	27 (2%) 53 43	2, 26, 61, 106	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	225	ALA	6.7
1	A	81	SER	5.8
1	C	1	SER	4.6
1	C	284	LEU	4.2
1	A	56	THR	4.1
1	B	56	THR	3.9
1	C	56	THR	3.6
1	C	81	SER	3.4
1	A	57	ARG	3.4
1	C	281	GLN	3.1
1	C	282	THR	3.0
1	A	280	ASP	2.9
1	A	204	LEU	2.9
1	A	249	LEU	2.9
1	C	287	LYS	2.8
1	A	86	LYS	2.6
1	A	246	ARG	2.4
1	A	215	THR	2.4
1	A	85	HIS	2.3
1	C	161	ALA	2.2
1	B	1	SER	2.2
1	B	81	SER	2.1
1	C	267	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	234	VAL	2.0
1	B	333	LYS	2.0
1	B	80	GLY	2.0
1	B	79	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.