



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:56 AM UTC

PDB ID : 3BGT / pdb_00003bgt
Title : Structural Studies of Acetoacetate Decarboxylase
Authors : Ho, M.; Allen, K.N.
Deposited on : 2007-11-27
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

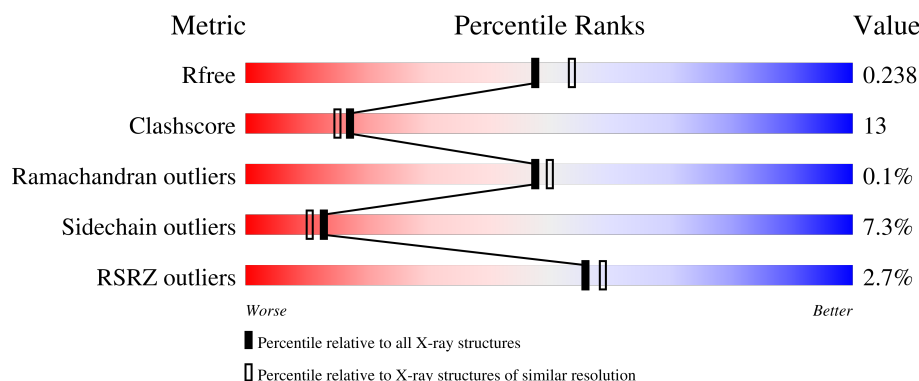
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	0% 70% 24% 0% ..
1	B	246	2% 76% 19% 0% ..
1	C	246	2% 75% 19% 6% .
1	D	246	4% 72% 22% 0% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8082 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 Probable acetoacetate decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	244	Total	C	N	O	S	Se	0	2	0
			1924	1241	327	346	2	8			
1	B	244	Total	C	N	O	S	Se	0	1	0
			1913	1235	323	345	2	8			
1	C	244	Total	C	N	O	S	Se	0	1	0
			1913	1235	323	345	2	8			
1	D	245	Total	C	N	O	S	Se	0	1	0
			1924	1241	327	346	2	8			

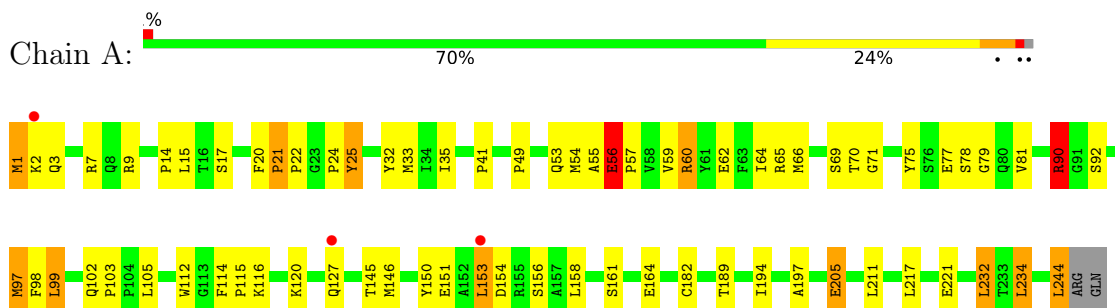
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	114	Total	O	0	0
			114	114		
2	B	122	Total	O	0	0
			122	122		
2	C	86	Total	O	0	0
			86	86		
2	D	86	Total	O	0	0
			86	86		

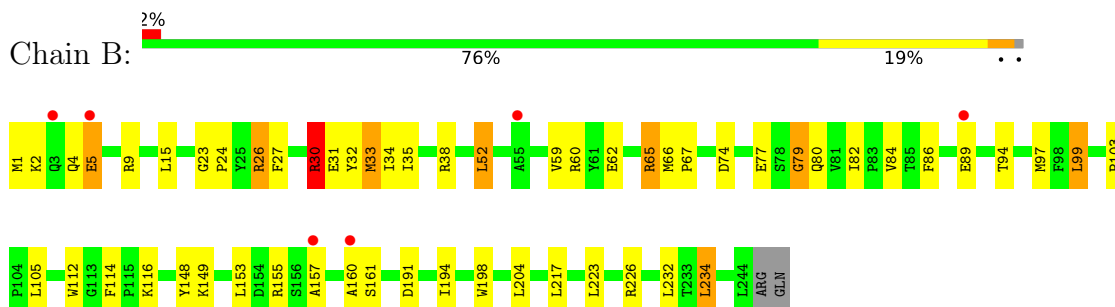
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

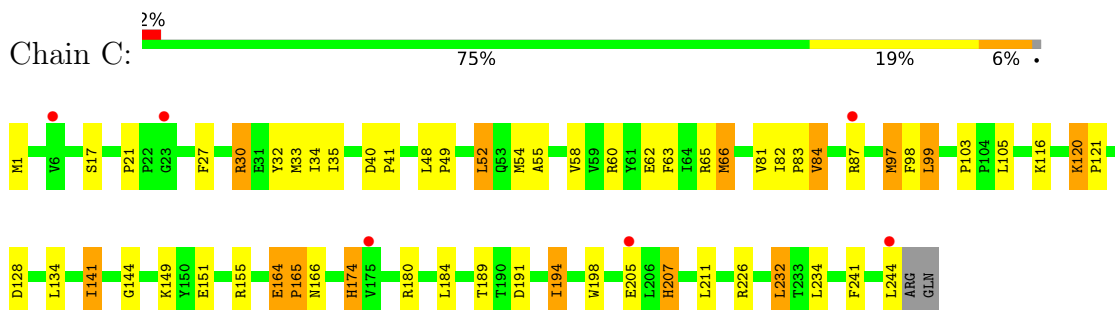
- Molecule 1: Probable acetoacetate decarboxylase



- Molecule 1: Probable acetoacetate decarboxylase

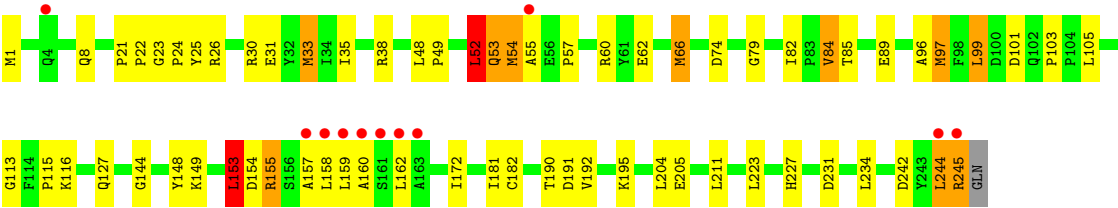


- Molecule 1: Probable acetoacetate decarboxylase



- Molecule 1: Probable acetoacetate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	105.45Å 105.45Å 252.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.30 – 2.10 30.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.30-2.10) 94.1 (30.30-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0005, CNS	Depositor
R, R_{free}	0.201 , 0.245 0.195 , 0.238	Depositor DCC
R_{free} test set	11784 reflections (8.81%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.009 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.004 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.002 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.005 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.003 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.020 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8082	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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	1.91	62/1972 (3.1%)	1.27	20/2677 (0.7%)
1	B	1.06	9/1961 (0.5%)	1.04	4/2663 (0.2%)
1	C	1.35	25/1961 (1.3%)	1.12	20/2663 (0.8%)
1	D	1.62	42/1972 (2.1%)	1.17	17/2677 (0.6%)
All	All	1.52	138/7866 (1.8%)	1.15	61/10680 (0.6%)

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	A	1	0

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	PHE	C-O	-18.23	1.04	1.24
1	A	102	GLN	N-CA	-16.74	1.35	1.46
1	D	62	GLU	C-O	-15.23	1.05	1.24
1	D	22	PRO	CA-C	-15.03	1.34	1.52
1	A	90	ARG	CB-CG	-14.88	1.07	1.52
1	A	70	THR	C-O	-14.35	1.06	1.23
1	C	98	PHE	C-O	-13.79	1.08	1.23
1	A	21	PRO	C-O	-13.65	1.09	1.24
1	C	191	ASP	C-O	-13.58	1.06	1.23
1	A	221	GLU	C-O	-13.41	1.07	1.24
1	D	53	GLN	C-O	-13.15	1.07	1.24
1	A	127	GLN	C-O	-13.06	1.07	1.24
1	A	3	GLN	C-O	-12.77	1.07	1.24
1	B	31	GLU	C-O	-12.70	1.08	1.24
1	D	22	PRO	CA-CB	-12.57	1.36	1.53
1	A	24	PRO	CG-CD	-12.54	1.17	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	22	PRO	C-O	-12.29	1.08	1.23
1	D	52	LEU	CA-C	-12.20	1.36	1.52
1	C	165	PRO	C-O	-12.19	1.10	1.23
1	C	97[A]	MSE	C-O	-11.96	1.09	1.23
1	C	97[B]	MSE	C-O	-11.96	1.09	1.23
1	C	205	GLU	C-O	-11.31	1.10	1.24
1	D	21	PRO	C-O	-11.29	1.11	1.24
1	A	22	PRO	C-O	-11.17	1.10	1.23
1	D	52	LEU	C-O	-11.13	1.10	1.23
1	A	90	ARG	CA-CB	-10.76	1.36	1.53
1	A	56	GLU	C-O	-10.62	1.10	1.24
1	C	87	ARG	C-O	-10.61	1.10	1.23
1	A	71	GLY	C-O	-10.48	1.08	1.24
1	D	155	ARG	N-CA	-10.34	1.33	1.46
1	D	54	MSE	N-CA	-10.07	1.33	1.46
1	C	97[A]	MSE	N-CA	-9.85	1.33	1.45
1	C	97[B]	MSE	N-CA	-9.85	1.33	1.45
1	D	54	MSE	CG-SE	9.79	2.24	1.95
1	A	90	ARG	C-O	-9.75	1.11	1.23
1	D	54	MSE	SE-CE	9.62	2.24	1.95
1	D	25	TYR	C-O	-9.62	1.10	1.23
1	D	54	MSE	CA-CB	-9.60	1.37	1.53
1	A	102	GLN	C-O	-9.59	1.16	1.24
1	D	23	GLY	C-O	-9.54	1.11	1.24
1	C	166	ASN	C-O	-9.39	1.12	1.24
1	A	60[A]	ARG	C-O	-9.33	1.11	1.23
1	A	60[B]	ARG	C-O	-9.33	1.11	1.23
1	D	97[A]	MSE	C-O	-9.33	1.12	1.23
1	D	97[B]	MSE	C-O	-9.33	1.12	1.23
1	D	54	MSE	C-O	-9.09	1.13	1.23
1	A	205	GLU	C-O	-9.02	1.13	1.24
1	B	89	GLU	CB-CG	-8.93	1.25	1.52
1	C	166	ASN	CG-ND2	-8.86	1.14	1.33
1	A	21	PRO	CA-CB	-8.83	1.42	1.54
1	A	62	GLU	C-O	-8.73	1.12	1.23
1	D	155	ARG	CZ-NH2	-8.67	1.22	1.33
1	D	53	GLN	CB-CG	-8.33	1.27	1.52
1	A	102	GLN	CD-OE1	-8.33	1.07	1.23
1	D	52	LEU	CG-CD1	-8.25	1.25	1.52
1	A	205	GLU	CB-CG	-8.23	1.27	1.52
1	D	22	PRO	CG-CD	-8.06	1.23	1.50
1	A	70	THR	CA-C	-7.95	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	116	LYS	C-O	-7.88	1.14	1.23
1	C	166	ASN	CG-OD1	-7.85	1.08	1.23
1	C	87	ARG	CA-C	-7.82	1.43	1.53
1	D	205	GLU	C-O	-7.81	1.14	1.23
1	B	31	GLU	CD-OE1	-7.75	1.10	1.25
1	A	90	ARG	CG-CD	-7.75	1.29	1.52
1	A	97[A]	MSE	C-N	-7.72	1.23	1.33
1	A	97[B]	MSE	C-N	-7.72	1.23	1.33
1	D	25	TYR	N-CA	-7.71	1.36	1.46
1	D	52	LEU	CG-CD2	-7.61	1.27	1.52
1	A	20	PHE	N-CA	-7.58	1.36	1.46
1	B	31	GLU	N-CA	-7.47	1.37	1.46
1	D	54	MSE	CB-CG	-7.46	1.30	1.52
1	D	53	GLN	CG-CD	-7.45	1.33	1.52
1	B	33	MSE	SE-CE	-7.42	1.73	1.95
1	A	102	GLN	CD-NE2	-7.41	1.17	1.33
1	A	62	GLU	CB-CG	-7.40	1.30	1.52
1	D	116	LYS	CG-CD	-7.37	1.30	1.52
1	A	22	PRO	CB-CG	-7.28	1.13	1.49
1	B	31	GLU	CD-OE2	-7.28	1.11	1.25
1	D	205	GLU	N-CA	-7.26	1.36	1.46
1	A	3	GLN	CA-C	-7.23	1.43	1.52
1	B	89	GLU	C-O	-7.19	1.15	1.24
1	C	205	GLU	N-CA	-6.84	1.37	1.46
1	A	24	PRO	C-O	-6.79	1.09	1.23
1	A	20	PHE	CE2-CZ	-6.77	1.18	1.38
1	B	31	GLU	CA-C	-6.71	1.44	1.52
1	A	22	PRO	CA-CB	-6.65	1.44	1.53
1	A	205	GLU	CD-OE2	-6.65	1.12	1.25
1	A	3	GLN	C-N	-6.60	1.24	1.33
1	C	165	PRO	N-CA	-6.58	1.39	1.47
1	A	22	PRO	CG-CD	-6.52	1.28	1.50
1	A	102	GLN	CA-C	-6.49	1.45	1.52
1	A	69	SER	C-O	-6.46	1.15	1.23
1	D	33	MSE	SE-CE	-6.45	1.76	1.95
1	C	191	ASP	C-N	-6.43	1.25	1.33
1	D	205	GLU	CD-OE1	-6.43	1.13	1.25
1	A	70	THR	C-N	-6.37	1.24	1.33
1	D	205	GLU	CD-OE2	-6.33	1.13	1.25
1	C	98	PHE	CE2-CZ	-6.33	1.19	1.38
1	A	20	PHE	CG-CD1	-6.32	1.25	1.38
1	A	57	PRO	C-O	-6.29	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60[A]	ARG	N-CA	-6.26	1.38	1.46
1	A	60[B]	ARG	N-CA	-6.26	1.38	1.46
1	A	57	PRO	CA-CB	-6.15	1.46	1.53
1	C	98	PHE	CG-CD2	-6.13	1.25	1.38
1	D	53	GLN	CA-C	-6.09	1.45	1.52
1	D	24	PRO	C-O	-6.01	1.11	1.23
1	D	155	ARG	C-O	-6.01	1.16	1.24
1	A	24	PRO	CA-CB	-5.99	1.43	1.53
1	A	57	PRO	C-N	-5.93	1.25	1.33
1	A	69	SER	CB-OG	-5.88	1.30	1.42
1	A	57	PRO	CA-C	-5.81	1.48	1.53
1	A	70	THR	CB-CG2	-5.78	1.33	1.52
1	A	151	GLU	C-O	-5.73	1.17	1.23
1	D	115	PRO	C-N	-5.66	1.25	1.33
1	C	87	ARG	C-N	-5.57	1.25	1.33
1	A	3	GLN	CA-CB	-5.51	1.44	1.53
1	C	205	GLU	CD-OE1	-5.50	1.15	1.25
1	C	166	ASN	CA-C	-5.46	1.46	1.52
1	A	69	SER	C-N	-5.43	1.26	1.33
1	A	21	PRO	CG-CD	-5.39	1.32	1.50
1	D	205	GLU	CA-C	-5.33	1.46	1.52
1	A	20	PHE	C-N	-5.33	1.27	1.33
1	C	165	PRO	CG-CD	-5.31	1.32	1.50
1	D	22	PRO	N-CA	-5.28	1.41	1.46
1	D	25	TYR	CZ-OH	-5.28	1.26	1.38
1	C	166	ASN	N-CA	-5.27	1.39	1.46
1	A	22	PRO	C-N	-5.26	1.25	1.33
1	A	102	GLN	C-N	-5.25	1.27	1.33
1	A	62	GLU	CD-OE2	-5.21	1.15	1.25
1	A	90	ARG	CA-C	-5.19	1.46	1.52
1	C	98	PHE	CG-CD1	-5.19	1.27	1.38
1	D	204	LEU	C-N	-5.18	1.25	1.33
1	A	22	PRO	N-CD	-5.15	1.40	1.47
1	A	57	PRO	N-CA	-5.13	1.39	1.48
1	B	89	GLU	N-CA	-5.10	1.39	1.46
1	D	62	GLU	CB-CG	-5.07	1.37	1.52
1	A	127	GLN	C-N	-5.05	1.26	1.33
1	C	191	ASP	CG-OD2	-5.03	1.15	1.25

All (61) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	ARG	N-CA-C	10.26	125.32	110.24
1	D	53	GLN	N-CA-C	9.67	125.17	109.40
1	D	62	GLU	N-CA-C	9.50	124.89	109.59
1	C	17	SER	CA-C-N	8.48	128.55	119.90
1	C	17	SER	C-N-CA	8.48	128.55	119.90
1	A	25	TYR	N-CA-C	8.01	123.04	107.98
1	D	153	LEU	CA-C-N	-7.87	110.24	121.50
1	D	153	LEU	C-N-CA	-7.87	110.24	121.50
1	D	155	ARG	NE-CZ-NH1	7.61	129.11	121.50
1	A	70	THR	N-CA-C	7.29	120.95	110.10
1	A	102	GLN	N-CA-C	7.26	122.04	112.17
1	D	155	ARG	N-CA-C	-6.94	103.15	111.69
1	D	55	ALA	N-CA-C	-6.82	99.68	109.29
1	A	21	PRO	N-CA-C	6.63	118.79	110.70
1	A	97[A]	MSE	O-C-N	6.58	131.13	123.17
1	A	97[B]	MSE	O-C-N	6.58	131.13	123.17
1	D	97[A]	MSE	CA-CB-CG	6.55	127.19	114.10
1	D	97[B]	MSE	CA-CB-CG	6.55	127.19	114.10
1	C	174	HIS	N-CA-C	-6.47	101.21	110.59
1	D	55	ALA	CB-CA-C	-6.32	106.50	114.40
1	B	30	ARG	N-CA-CB	6.23	119.22	109.69
1	D	54	MSE	N-CA-C	6.12	119.11	110.23
1	D	25	TYR	N-CA-C	6.06	119.39	108.17
1	C	21	PRO	CA-C-N	6.06	125.77	119.05
1	C	21	PRO	C-N-CA	6.06	125.77	119.05
1	A	90	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	C	207	HIS	CA-C-N	5.94	125.88	119.76
1	C	207	HIS	C-N-CA	5.94	125.88	119.76
1	C	55	ALA	N-CA-C	-5.90	100.97	109.29
1	A	21	PRO	CA-C-N	5.90	125.86	119.78
1	A	21	PRO	C-N-CA	5.90	125.86	119.78
1	A	75	TYR	N-CA-C	5.88	116.85	108.74
1	C	164	GLU	CA-C-N	5.76	125.52	119.76
1	C	164	GLU	C-N-CA	5.76	125.52	119.76
1	B	66	MSE	CG-SE-CE	-5.69	86.40	98.92
1	D	154	ASP	N-CA-CB	5.67	118.75	109.95
1	A	90	ARG	CB-CA-C	5.66	118.33	109.84
1	B	31	GLU	N-CA-C	5.58	117.61	108.52
1	A	102	GLN	N-CA-CB	5.55	115.67	110.39
1	C	103	PRO	N-CA-C	5.49	117.40	110.70
1	A	90	ARG	CB-CG-CD	-5.41	98.86	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	127	GLN	N-CA-C	-5.41	99.64	108.67
1	A	103	PRO	N-CA-C	5.31	117.18	110.70
1	A	21	PRO	O-C-N	5.28	127.69	121.46
1	A	62	GLU	CB-CG-CD	5.24	121.51	112.60
1	C	66	MSE	CG-SE-CE	-5.23	87.41	98.92
1	C	40	ASP	CA-C-N	5.21	125.26	119.32
1	C	40	ASP	C-N-CA	5.21	125.26	119.32
1	D	54	MSE	N-CA-CB	-5.18	102.01	109.83
1	A	70	THR	N-CA-CB	5.16	117.59	109.69
1	B	79	GLY	N-CA-C	5.15	118.22	110.18
1	D	155	ARG	NE-CZ-NH2	-5.13	114.59	119.20
1	C	97[A]	MSE	CA-C-N	5.08	129.91	122.39
1	C	97[A]	MSE	C-N-CA	5.08	129.91	122.39
1	C	97[B]	MSE	CA-C-N	5.08	129.91	122.39
1	C	97[B]	MSE	C-N-CA	5.08	129.91	122.39
1	D	53	GLN	CB-CA-C	-5.06	99.70	109.37
1	A	57	PRO	CA-N-CD	-5.05	104.92	112.00
1	A	90	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	C	30	ARG	N-CA-C	-5.02	102.95	110.23
1	C	55	ALA	CB-CA-C	-5.01	108.13	114.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	90	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1924	0	1923	59	3
1	B	1913	0	1911	55	0
1	C	1913	0	1911	42	0
1	D	1924	0	1924	41	0
2	A	114	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	122	0	0	3	0
2	C	86	0	0	2	3
2	D	86	0	0	5	0
All	All	8082	0	7669	194	3

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 13.

All (194) 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:B:77:GLU:HG2	1:B:97[B]:MSE:CE	1.51	1.38
1:D:54:MSE:SE	1:D:54:MSE:CG	2.24	1.36
1:A:77:GLU:HG2	1:A:97[B]:MSE:CE	1.56	1.35
1:D:54:MSE:SE	1:D:54:MSE:CE	2.24	1.35
1:A:77:GLU:CG	1:A:97[B]:MSE:HE3	1.66	1.24
1:A:97[A]:MSE:HE1	1:A:114:PHE:CD1	1.80	1.17
1:A:33:MSE:HE2	1:A:35:ILE:HD11	1.32	1.10
1:A:79:GLY:HA3	1:A:97[B]:MSE:SE	2.00	1.10
1:A:77:GLU:CG	1:A:97[B]:MSE:CE	2.27	1.10
1:C:226:ARG:NH1	2:C:331:HOH:O	1.84	1.08
1:A:205:GLU:OE1	2:A:331:HOH:O	1.72	1.05
1:A:33:MSE:HE3	1:A:146:MSE:HG3	1.38	1.05
1:B:77:GLU:HG2	1:B:97[B]:MSE:HE3	1.10	1.05
1:B:77:GLU:CG	1:B:97[B]:MSE:CE	2.35	1.05
1:B:77:GLU:HG2	1:B:97[B]:MSE:HE2	1.37	1.04
1:B:1:MSE:HE3	1:B:15:LEU:HD23	1.41	1.02
1:B:94:THR:HG21	1:B:97[A]:MSE:HE3	1.41	1.02
1:A:77:GLU:HG2	1:A:97[B]:MSE:HE3	1.29	0.99
1:B:34:ILE:HD12	1:B:62:GLU:HG2	1.41	0.99
1:A:77:GLU:HG2	1:A:97[B]:MSE:HE1	1.44	0.99
1:B:153:LEU:HD21	1:B:226:ARG:HD2	1.43	0.97
1:B:77:GLU:CG	1:B:97[B]:MSE:HE3	1.94	0.95
1:C:33:MSE:HE3	1:C:35:ILE:CD1	1.98	0.94
1:B:1:MSE:HE3	1:B:15:LEU:CD2	1.97	0.94
1:B:77:GLU:CG	1:B:97[B]:MSE:HE2	1.98	0.93
1:C:33:MSE:HE2	1:C:63:PHE:HD2	1.33	0.92
1:C:33:MSE:HE3	1:C:35:ILE:HD12	1.50	0.92
1:D:48:LEU:HD13	1:D:82:ILE:HD11	1.50	0.91
1:C:33:MSE:HE2	1:C:63:PHE:CD2	2.05	0.90
1:A:56:GLU:OE1	1:A:90:ARG:NH2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:MSE:CE	1:A:35:ILE:HD11	2.04	0.87
1:A:77:GLU:HG3	1:A:97[B]:MSE:HE3	1.58	0.83
1:A:97[A]:MSE:CE	1:A:114:PHE:HB3	2.08	0.83
1:A:97[A]:MSE:HE1	1:A:114:PHE:CG	2.13	0.82
1:A:153:LEU:HD22	1:A:197:ALA:HB1	1.59	0.82
1:B:77:GLU:CD	1:B:97[B]:MSE:HE2	2.05	0.81
1:D:113:GLY:O	2:D:254:HOH:O	1.99	0.79
1:B:1:MSE:CE	1:B:15:LEU:HD23	2.12	0.79
1:A:33:MSE:HE2	1:A:35:ILE:CD1	2.12	0.78
1:D:96:ALA:O	1:D:97[A]:MSE:HE2	1.82	0.78
1:A:154:ASP:OD2	2:A:294:HOH:O	2.03	0.77
1:D:8:GLN:O	2:D:322:HOH:O	2.04	0.76
1:A:97[A]:MSE:CE	1:A:114:PHE:CD1	2.65	0.75
1:B:34:ILE:CD1	1:B:62:GLU:HG2	2.16	0.75
1:D:79:GLY:HA3	1:D:97[A]:MSE:HE2	1.68	0.74
1:B:77:GLU:OE2	1:B:97[B]:MSE:HE2	1.87	0.74
1:D:26:ARG:HH12	1:D:191:ASP:HB3	1.54	0.72
1:D:79:GLY:HA3	1:D:97[A]:MSE:CE	2.20	0.71
1:A:97[A]:MSE:HE1	1:A:114:PHE:HB3	1.72	0.71
1:C:33:MSE:CE	1:C:35:ILE:HD12	2.20	0.71
1:A:153:LEU:HD22	1:A:197:ALA:CB	2.20	0.70
1:A:32:TYR:CD2	1:A:64:ILE:HD12	2.27	0.69
1:C:33:MSE:CE	1:C:63:PHE:CD2	2.74	0.69
1:A:97[A]:MSE:HE1	1:A:114:PHE:HD1	1.49	0.69
1:B:38:ARG:HB2	1:B:223:LEU:HD11	1.73	0.69
1:B:79:GLY:HA3	1:B:97[B]:MSE:SE	2.43	0.68
1:A:158:LEU:HD23	1:A:194:ILE:HD13	1.76	0.67
1:D:33:MSE:HE3	1:D:35:ILE:HD11	1.77	0.67
1:D:99:LEU:CD1	1:D:105:LEU:HG	2.25	0.67
1:C:34:ILE:HD12	1:C:62:GLU:HG2	1.78	0.66
1:A:97[A]:MSE:CE	1:A:114:PHE:HD1	2.07	0.66
1:B:60:ARG:HD2	2:B:299:HOH:O	1.96	0.66
1:A:97[A]:MSE:HE1	1:A:114:PHE:CB	2.27	0.65
1:A:153:LEU:CD2	1:A:197:ALA:HB1	2.26	0.65
1:B:157:ALA:O	1:B:160:ALA:HB3	1.97	0.65
1:A:77:GLU:CD	1:A:97[B]:MSE:CE	2.70	0.64
1:B:26:ARG:NH2	1:B:191:ASP:O	2.30	0.64
1:C:33:MSE:CE	1:C:35:ILE:CD1	2.77	0.62
1:D:33:MSE:HE1	1:D:144:GLY:C	2.24	0.62
1:A:97[A]:MSE:HE2	1:A:115:PRO:HD2	1.82	0.62
1:C:27:PHE:HB3	1:C:30:ARG:HD3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MSE:HA	1:B:5:GLU:OE2	2.00	0.62
1:D:60:ARG:NH2	2:D:327:HOH:O	2.33	0.61
1:A:49:PRO:HA	1:B:1:MSE:HG2	1.81	0.61
1:B:94:THR:CG2	1:B:97[A]:MSE:HE3	2.24	0.61
1:B:99:LEU:HD11	1:B:116:LYS:HG2	1.81	0.61
1:C:149:LYS:HD3	1:C:198:TRP:CE2	2.37	0.60
1:A:97[A]:MSE:HE3	1:A:114:PHE:HB3	1.82	0.59
1:A:97[A]:MSE:HE3	1:A:116:LYS:HG3	1.85	0.59
1:B:99:LEU:HD13	1:B:105:LEU:HG	1.83	0.59
1:C:99:LEU:HD13	1:C:105:LEU:HG	1.85	0.59
1:C:33:MSE:HE1	1:C:144:GLY:HA3	1.85	0.58
1:C:32:TYR:HD2	1:C:34:ILE:HD11	1.69	0.58
1:B:155:ARG:HG2	1:B:194:ILE:HG21	1.84	0.58
1:C:120:LYS:HG3	1:C:120:LYS:O	2.03	0.58
1:C:49:PRO:O	1:C:52:LEU:HB2	2.03	0.57
1:D:242:ASP:O	1:D:245:ARG:HG3	2.05	0.57
1:D:182:CYS:HB3	1:D:244:LEU:HD13	1.86	0.56
1:B:59:VAL:HG11	1:B:80:GLN:HG2	1.87	0.55
1:C:134:LEU:HG	1:C:141:ILE:HD11	1.88	0.55
1:D:38:ARG:HB2	1:D:223:LEU:HD11	1.87	0.54
1:C:65:ARG:HD3	2:C:258:HOH:O	2.07	0.54
1:A:189:THR:HB	1:A:232:LEU:HG	1.90	0.54
1:B:33:MSE:O	1:B:34:ILE:HD13	2.08	0.53
1:A:77:GLU:CD	1:A:97[B]:MSE:HE2	2.33	0.53
1:A:1:MSE:HE1	1:A:15:LEU:HD21	1.91	0.53
1:C:33:MSE:HE3	1:C:35:ILE:HD11	1.87	0.53
1:D:99:LEU:HD11	1:D:105:LEU:HG	1.91	0.53
1:B:148:TYR:CE2	1:B:149:LYS:HD2	2.43	0.53
1:C:27:PHE:CB	1:C:30:ARG:HD3	2.39	0.52
1:A:99:LEU:HD13	1:A:105:LEU:HG	1.91	0.52
1:B:65:ARG:HH11	1:B:65:ARG:HB3	1.73	0.52
1:C:155:ARG:NE	1:C:194:ILE:HD11	2.25	0.52
1:C:60:ARG:HH21	1:C:83:PRO:HB3	1.75	0.51
1:B:153:LEU:CD2	1:B:226:ARG:HD2	2.30	0.51
1:A:77:GLU:CD	1:A:97[B]:MSE:HE3	2.30	0.50
1:A:41:PRO:HB3	1:A:54:MSE:HE1	1.93	0.50
1:B:34:ILE:HD12	1:B:62:GLU:CG	2.29	0.50
1:B:74:ASP:C	1:B:74:ASP:OD1	2.54	0.50
1:B:99:LEU:HD11	1:B:116:LYS:CG	2.40	0.50
1:C:164:GLU:HB3	1:C:165:PRO:HD2	1.93	0.50
1:D:148:TYR:CE2	1:D:149:LYS:HD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:PHE:HB2	1:C:232:LEU:HD22	1.94	0.49
1:B:35:ILE:HG21	1:B:204:LEU:HB2	1.93	0.49
1:C:33:MSE:HE1	1:C:63:PHE:CE2	2.48	0.49
1:A:153:LEU:CD2	1:A:197:ALA:CB	2.87	0.49
1:A:33:MSE:HE1	1:A:145:THR:N	2.28	0.48
1:B:112:TRP:CZ2	1:B:234:LEU:HD13	2.47	0.48
1:C:164:GLU:HB3	1:C:165:PRO:CD	2.42	0.48
1:A:182:CYS:HB3	1:A:244:LEU:HD13	1.95	0.48
1:B:59:VAL:CG1	1:B:80:GLN:HG2	2.44	0.47
1:C:62:GLU:OE1	1:C:97[B]:MSE:HE1	2.14	0.47
1:D:54:MSE:HE1	1:D:57:PRO:HB3	1.97	0.47
1:B:33:MSE:C	1:B:34:ILE:HD13	2.40	0.47
1:B:52:LEU:HD12	1:B:86:PHE:HB2	1.97	0.47
1:D:99:LEU:HD12	1:D:99:LEU:H	1.80	0.47
1:B:1:MSE:HA	1:B:5:GLU:CD	2.40	0.47
1:B:82:ILE:HD11	1:B:217:LEU:HD21	1.98	0.46
1:D:97[B]:MSE:CE	2:D:332:HOH:O	2.64	0.46
1:A:33:MSE:HE2	1:A:35:ILE:CG1	2.45	0.46
1:A:97[B]:MSE:C	1:A:98:PHE:CD2	2.94	0.46
1:A:54:MSE:HG2	1:A:55:ALA:O	2.16	0.46
1:A:97[A]:MSE:C	1:A:98:PHE:CD2	2.94	0.46
1:B:149:LYS:HG2	1:B:198:TRP:CD2	2.51	0.45
1:D:153:LEU:HD12	1:D:153:LEU:HA	1.50	0.45
1:A:161:SER:O	1:A:164:GLU:HG2	2.16	0.45
1:D:195:LYS:HE3	1:D:231:ASP:OD1	2.16	0.45
1:C:99:LEU:HD11	1:C:116:LYS:HD3	1.98	0.45
1:B:60:ARG:NH2	2:B:345:HOH:O	2.15	0.45
1:C:174:HIS:HB2	1:C:180:ARG:HB2	1.99	0.44
1:A:81:VAL:CG1	1:A:92:SER:HB2	2.46	0.44
1:A:99:LEU:HD11	1:A:116:LYS:HD3	1.99	0.44
1:D:85:THR:HA	1:D:89:GLU:O	2.17	0.44
1:B:23:GLY:CA	1:B:24:PRO:C	2.91	0.44
1:C:120:LYS:HE2	1:C:121:PRO:O	2.18	0.44
1:C:189:THR:HB	1:C:232:LEU:HG	2.00	0.44
1:B:65:ARG:HH12	1:B:67:PRO:N	2.15	0.44
1:C:141:ILE:HA	1:C:207:HIS:HB2	2.00	0.44
1:A:59:VAL:HG21	1:A:217:LEU:HD23	2.00	0.43
1:C:58:VAL:HG22	1:C:83:PRO:HG3	2.01	0.43
1:D:49:PRO:O	1:D:52:LEU:HB2	2.18	0.43
1:D:48:LEU:CD1	1:D:82:ILE:HD11	2.35	0.43
1:D:31:GLU:OE2	1:D:227:HIS:NE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLY:CA	1:D:97[A]:MSE:CE	2.93	0.43
1:C:184:LEU:HB2	1:C:241:PHE:HB3	2.01	0.43
1:B:26:ARG:NH2	1:B:191:ASP:HB3	2.34	0.43
1:D:48:LEU:HD21	1:D:84:VAL:HG23	2.00	0.43
1:C:41:PRO:HA	1:C:54:MSE:HE1	2.01	0.43
1:C:99:LEU:HD11	1:C:116:LYS:CG	2.49	0.43
1:D:97[B]:MSE:HE1	2:D:332:HOH:O	2.17	0.43
1:D:99:LEU:HD12	1:D:99:LEU:N	2.34	0.43
1:A:49:PRO:HD3	1:B:1:MSE:HE2	2.01	0.42
1:B:26:ARG:HH21	1:B:191:ASP:HB3	1.84	0.42
1:C:33:MSE:CE	1:C:63:PHE:CE2	3.02	0.42
1:B:82:ILE:HD11	1:B:217:LEU:CD2	2.49	0.42
1:D:26:ARG:NH1	1:D:191:ASP:HB3	2.29	0.42
1:A:77:GLU:OE2	1:A:99:LEU:HG	2.19	0.42
1:D:79:GLY:C	1:D:97[A]:MSE:HE1	2.44	0.42
1:A:14:PRO:HD2	1:A:17:SER:O	2.20	0.42
1:A:56:GLU:H	1:A:56:GLU:HG3	1.42	0.42
1:A:112:TRP:CZ2	1:A:234:LEU:HD13	2.54	0.42
1:B:97[A]:MSE:HE1	1:B:114:PHE:CE1	2.55	0.42
1:D:74:ASP:OD1	1:D:74:ASP:C	2.63	0.42
1:C:48:LEU:HD11	1:C:84:VAL:HG23	2.02	0.42
1:C:164:GLU:CB	1:C:165:PRO:CD	2.95	0.42
1:D:99:LEU:HD13	1:D:105:LEU:HG	2.01	0.42
1:A:156:SER:HB2	2:A:294:HOH:O	2.19	0.41
1:B:27:PHE:CB	1:B:30:ARG:HD3	2.51	0.41
1:D:162:LEU:HD12	1:D:192:VAL:HG11	2.01	0.41
1:D:172:ILE:HG13	1:D:181:ILE:HD12	2.02	0.41
1:B:103:PRO:HG2	1:C:128:ASP:CB	2.51	0.41
1:D:30:ARG:NH1	1:D:66:MSE:HE3	2.36	0.41
1:A:90:ARG:C	1:A:90:ARG:HD3	2.46	0.41
1:B:2:LYS:O	1:B:5:GLU:HB3	2.21	0.41
1:A:33:MSE:HE3	1:A:146:MSE:CG	2.29	0.41
1:B:24:PRO:HA	2:B:254:HOH:O	2.20	0.41
1:B:32:TYR:HD2	1:B:34:ILE:HD11	1.86	0.41
1:D:157:ALA:O	1:D:160:ALA:HB3	2.21	0.41
1:D:190:THR:O	1:D:191:ASP:HB2	2.21	0.41
1:A:78:SER:O	1:A:97[B]:MSE:HA	2.21	0.41
1:C:155:ARG:HD2	1:C:194:ILE:HG12	2.03	0.41
1:C:164:GLU:HA	1:C:165:PRO:HD3	1.71	0.41
1:A:79:GLY:CA	1:A:97[B]:MSE:SE	2.94	0.40
1:D:101:ASP:OD1	1:D:103:PRO:HD2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TYR:OH	2:C:301:HOH:O[2_765]	0.18	2.02
1:A:150:TYR:CZ	2:C:301:HOH:O[2_765]	1.17	1.03
1:A:150:TYR:CE2	2:C:301:HOH:O[2_765]	2.14	0.06

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	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
1	B	243/246 (99%)	233 (96%)	10 (4%)	0	100	100
1	C	243/246 (99%)	233 (96%)	10 (4%)	0	100	100
1	D	244/246 (99%)	233 (96%)	10 (4%)	1 (0%)	30	28
All	All	974/984 (99%)	935 (96%)	38 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	159	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	205/198 (104%)	185 (90%)	20 (10%)	7	5
1	B	204/198 (103%)	192 (94%)	12 (6%)	18	16
1	C	204/198 (103%)	189 (93%)	15 (7%)	13	10
1	D	205/198 (104%)	192 (94%)	13 (6%)	16	14
All	All	818/792 (103%)	758 (93%)	60 (7%)	13	10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	2	LYS
1	A	7	ARG
1	A	9	ARG
1	A	21	PRO
1	A	25	TYR
1	A	53	GLN
1	A	56	GLU
1	A	60[A]	ARG
1	A	60[B]	ARG
1	A	65	ARG
1	A	66	MSE
1	A	90	ARG
1	A	99	LEU
1	A	120	LYS
1	A	153	LEU
1	A	211	LEU
1	A	232	LEU
1	A	234	LEU
1	A	244	LEU
1	B	4	GLN
1	B	5	GLU
1	B	9	ARG
1	B	26	ARG
1	B	30	ARG
1	B	52	LEU
1	B	65	ARG
1	B	84	VAL
1	B	99	LEU
1	B	161	SER
1	B	232	LEU
1	B	234	LEU
1	C	1	MSE

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Mol	Chain	Res	Type
1	C	52	LEU
1	C	66	MSE
1	C	81	VAL
1	C	82	ILE
1	C	84	VAL
1	C	99	LEU
1	C	120	LYS
1	C	141	ILE
1	C	151	GLU
1	C	194	ILE
1	C	211	LEU
1	C	232	LEU
1	C	234	LEU
1	C	244	LEU
1	D	1	MSE
1	D	52	LEU
1	D	53	GLN
1	D	66	MSE
1	D	84	VAL
1	D	99	LEU
1	D	153	LEU
1	D	155	ARG
1	D	158	LEU
1	D	211	LEU
1	D	234	LEU
1	D	244	LEU
1	D	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	127	GLN
1	A	166	ASN
1	B	3	GLN
1	B	4	GLN
1	B	102	GLN
1	B	127	GLN
1	B	166	ASN
1	C	8	GLN
1	D	102	GLN
1	D	126	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/246 (96%)	-0.05	3 (1%) 75 77	13, 31, 48, 71	4 (1%)
1	B	237/246 (96%)	-0.07	6 (2%) 58 61	14, 29, 54, 68	3 (1%)
1	C	237/246 (96%)	0.20	6 (2%) 58 61	20, 37, 57, 79	2 (0%)
1	D	238/246 (96%)	0.39	11 (4%) 37 39	19, 39, 63, 80	2 (0%)
All	All	949/984 (96%)	0.12	26 (2%) 56 59	13, 34, 57, 80	11 (1%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	157	ALA	4.2
1	D	160	ALA	3.6
1	D	55	ALA	3.5
1	B	89	GLU	3.1
1	D	159	LEU	2.8
1	C	244	LEU	2.6
1	D	244	LEU	2.6
1	A	127	GLN	2.6
1	D	161	SER	2.6
1	D	245	ARG	2.6
1	B	5	GLU	2.5
1	A	153	LEU	2.5
1	B	3	GLN	2.5
1	B	55	ALA	2.5
1	C	87	ARG	2.5
1	C	23	GLY	2.3
1	D	4	GLN	2.3
1	C	205	GLU	2.3
1	D	157	ALA	2.3
1	D	158	LEU	2.2
1	D	162	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	2.1
1	B	160	ALA	2.1
1	A	2	LYS	2.1
1	C	175	VAL	2.0
1	D	163	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.