



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:06 AM UTC

PDB ID : 3G4H / pdb_00003g4h
Title : Crystal structure of Human Senescence Marker Protein-30 (Zinc Bound)
Authors : Chakraborti, S.; Bahnson, B.J.
Deposited on : 2009-02-03
Resolution : 1.92 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

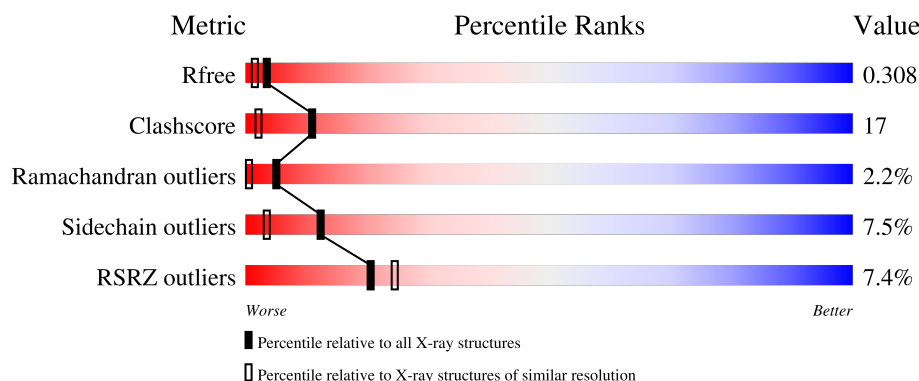
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	297	
1	B	297	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4752 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 Regucalcin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	297	Total	C	N	O	S	0	0	0
			2303	1455	395	438	15			
1	A	297	Total	C	N	O	S	0	0	0
			2303	1455	395	438	15			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

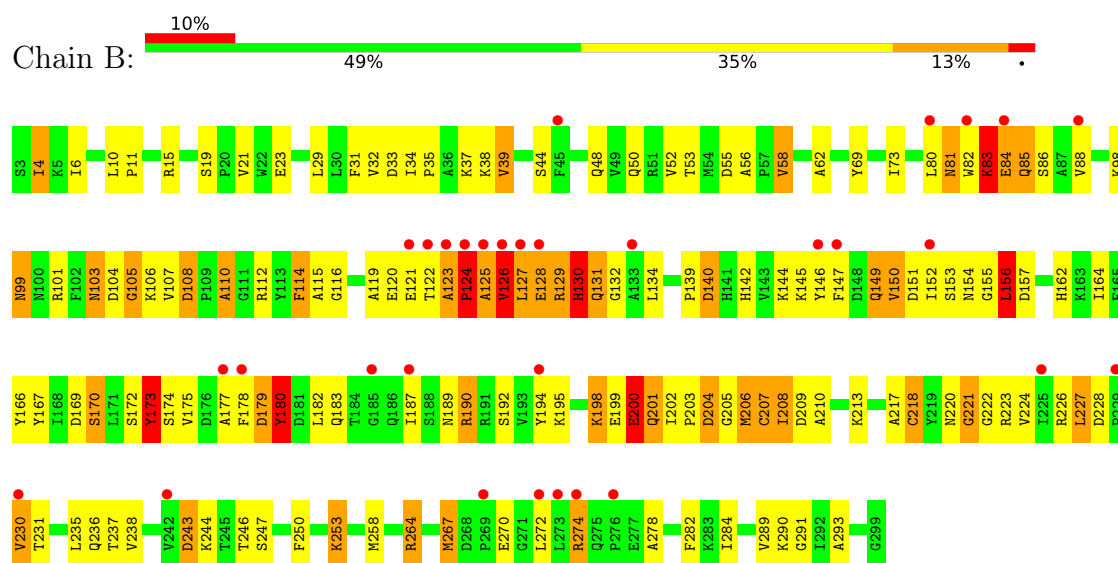
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	60	Total	O	0	0
			60	60		
3	A	84	Total	O	0	0
			84	84		

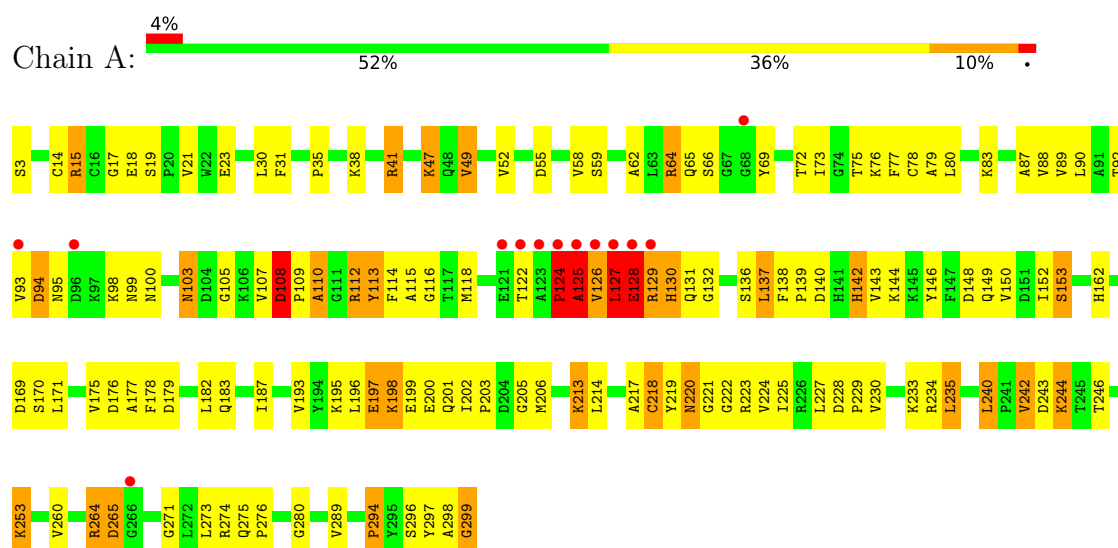
3 Residue-property plots [i](#)

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: Regucalcin



• Molecule 1: Regucalcin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.36Å 52.02Å 85.83Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	84.52 – 1.92 84.50 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.2 (84.52-1.92) 99.3 (84.50-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.253 0.239 , 0.308	Depositor DCC
R_{free} test set	2148 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4752	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	2.44	109/2353 (4.6%)	1.84	41/3185 (1.3%)
1	B	2.29	96/2353 (4.1%)	1.72	31/3185 (1.0%)
All	All	2.37	205/4706 (4.4%)	1.78	72/6370 (1.1%)

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	0	5
1	B	0	5
All	All	0	10

All (205) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLU	C-N	22.90	1.62	1.33
1	B	150	VAL	CA-CB	18.22	1.74	1.54
1	A	150	VAL	CA-CB	16.79	1.74	1.54
1	A	127	LEU	C-N	15.07	1.52	1.33
1	B	243	ASP	C-O	13.99	1.41	1.24
1	B	128	GLU	C-N	12.65	1.53	1.33
1	B	177	ALA	C-O	12.37	1.39	1.23
1	B	155	GLY	N-CA	12.16	1.60	1.45
1	B	175	VAL	CA-CB	11.86	1.69	1.54
1	B	203	PRO	C-O	11.83	1.37	1.23
1	A	103	ASN	C-O	10.48	1.31	1.23
1	A	246	THR	C-N	10.17	1.46	1.33
1	A	49	VAL	CA-CB	10.13	1.67	1.54
1	A	64	ARG	CA-C	9.94	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLY	N-CA	9.77	1.58	1.45
1	A	83	LYS	C-O	9.75	1.35	1.24
1	A	280	GLY	N-CA	9.36	1.57	1.45
1	A	89	VAL	N-CA	8.81	1.56	1.46
1	A	203	PRO	N-CA	8.72	1.56	1.46
1	B	103	ASN	C-O	8.69	1.29	1.23
1	A	225	ILE	CA-CB	8.68	1.67	1.54
1	A	92	THR	N-CA	8.61	1.56	1.45
1	A	297	TYR	CA-C	8.49	1.63	1.52
1	A	233	LYS	CA-C	8.47	1.62	1.52
1	B	114	PHE	C-O	8.43	1.34	1.23
1	A	108	ASP	CB-CG	-8.42	1.30	1.52
1	A	197	GLU	C-O	8.38	1.34	1.23
1	A	107	VAL	CA-CB	8.37	1.64	1.54
1	A	66	SER	C-O	-8.36	1.13	1.24
1	A	176	ASP	N-CA	8.36	1.55	1.45
1	B	223	ARG	NE-CZ	8.30	1.42	1.33
1	A	100	ASN	C-O	8.29	1.34	1.23
1	B	204	ASP	CA-C	8.25	1.63	1.52
1	A	143	VAL	CA-C	8.08	1.62	1.52
1	B	201	GLN	C-N	7.92	1.41	1.33
1	B	149	GLN	CD-OE1	7.82	1.38	1.23
1	A	169	ASP	C-O	7.71	1.33	1.24
1	A	128	GLU	C-O	-7.60	1.16	1.23
1	A	38	LYS	N-CA	7.42	1.55	1.46
1	B	208	ILE	CA-C	7.41	1.60	1.53
1	B	156	LEU	CA-C	7.39	1.62	1.52
1	A	126	VAL	C-O	7.38	1.32	1.24
1	A	62	ALA	CA-C	7.36	1.61	1.52
1	A	223	ARG	C-O	7.34	1.32	1.23
1	A	229	PRO	CA-C	7.31	1.64	1.52
1	B	103	ASN	CA-CB	7.29	1.66	1.52
1	B	206	MET	CG-SD	7.25	1.98	1.80
1	B	227	LEU	CG-CD2	7.25	1.76	1.52
1	A	149	GLN	N-CA	7.20	1.57	1.46
1	B	206	MET	C-N	7.14	1.42	1.33
1	B	33	ASP	CA-C	7.13	1.63	1.53
1	A	177	ALA	C-O	7.10	1.32	1.23
1	A	132	GLY	C-O	7.09	1.33	1.23
1	A	217	ALA	CA-C	7.06	1.61	1.52
1	B	19	SER	N-CA	7.04	1.52	1.46
1	A	73	ILE	CA-CB	7.02	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CYS	N-CA	6.97	1.54	1.45
1	A	113	TYR	CA-C	6.97	1.61	1.52
1	A	271	GLY	N-CA	6.96	1.54	1.45
1	A	52	VAL	CA-C	6.95	1.60	1.52
1	A	114	PHE	N-CA	6.94	1.54	1.46
1	A	218	CYS	N-CA	6.91	1.55	1.46
1	A	75	THR	CA-CB	6.91	1.62	1.53
1	B	52	VAL	C-O	6.91	1.31	1.24
1	A	175	VAL	CA-CB	6.83	1.62	1.54
1	B	205	GLY	C-N	6.75	1.41	1.33
1	B	170	SER	CA-C	6.75	1.62	1.52
1	B	164	ILE	C-O	6.74	1.30	1.23
1	B	180	TYR	CD1-CE1	6.69	1.58	1.38
1	B	115	ALA	CA-CB	6.63	1.64	1.53
1	B	116	GLY	N-CA	-6.57	1.38	1.44
1	A	193	VAL	CA-CB	6.56	1.62	1.54
1	B	108	ASP	CB-CG	-6.55	1.35	1.52
1	A	220	ASN	CG-ND2	6.49	1.46	1.33
1	B	29	LEU	C-O	6.45	1.31	1.24
1	A	72	THR	CA-CB	6.44	1.62	1.53
1	B	167	TYR	C-O	6.41	1.31	1.23
1	A	289	VAL	CA-C	6.38	1.60	1.52
1	B	149	GLN	CD-NE2	6.36	1.46	1.33
1	B	206	MET	C-O	-6.36	1.17	1.23
1	A	15	ARG	CB-CG	6.34	1.71	1.52
1	A	66	SER	CB-OG	6.32	1.54	1.42
1	B	132	GLY	N-CA	6.30	1.53	1.44
1	B	218	CYS	C-O	6.30	1.31	1.23
1	B	293	ALA	CA-C	6.30	1.60	1.53
1	A	108	ASP	CA-CB	6.29	1.63	1.53
1	A	105	GLY	CA-C	6.26	1.58	1.51
1	A	47	LYS	CG-CD	6.26	1.71	1.52
1	A	142	HIS	CA-C	6.25	1.61	1.52
1	A	17	GLY	N-CA	6.23	1.54	1.45
1	A	146	TYR	C-O	-6.22	1.16	1.24
1	A	271	GLY	CA-C	6.22	1.58	1.52
1	A	31	PHE	CA-C	-6.21	1.45	1.52
1	A	203	PRO	C-O	6.20	1.30	1.23
1	A	176	ASP	CA-C	6.19	1.61	1.53
1	A	171	LEU	N-CA	6.17	1.54	1.46
1	B	202	ILE	N-CA	6.17	1.51	1.46
1	A	125	ALA	C-N	6.12	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	MET	SD-CE	6.12	1.94	1.79
1	B	104	ASP	CB-CG	6.10	1.67	1.52
1	B	140	ASP	CG-OD2	6.10	1.36	1.25
1	A	19	SER	C-N	6.09	1.40	1.33
1	B	247	SER	CB-OG	6.08	1.54	1.42
1	B	228	ASP	C-O	6.07	1.32	1.24
1	B	253	LYS	CG-CD	6.06	1.70	1.52
1	B	6	ILE	N-CA	6.04	1.53	1.46
1	B	128	GLU	C-O	-6.04	1.16	1.24
1	A	66	SER	N-CA	6.03	1.54	1.46
1	B	210	ALA	CA-C	6.03	1.60	1.52
1	B	217	ALA	CA-CB	6.00	1.62	1.53
1	A	21	VAL	C-O	-5.98	1.18	1.24
1	A	83	LYS	CA-CB	5.93	1.62	1.53
1	B	62	ALA	CA-CB	5.92	1.64	1.53
1	B	202	ILE	CA-CB	5.92	1.60	1.53
1	B	237	THR	CA-C	5.92	1.59	1.52
1	A	142	HIS	N-CA	5.92	1.53	1.45
1	B	108	ASP	CA-CB	5.91	1.62	1.53
1	A	294	PRO	CB-CG	5.89	1.79	1.49
1	B	130	HIS	N-CA	5.83	1.53	1.46
1	B	221	GLY	C-O	5.82	1.30	1.24
1	A	253	LYS	C-O	5.81	1.30	1.24
1	B	238	VAL	C-O	5.78	1.30	1.24
1	A	59	SER	N-CA	5.74	1.53	1.46
1	A	138	PHE	CA-C	5.74	1.60	1.53
1	A	131	GLN	CA-C	5.73	1.60	1.52
1	A	213	LYS	C-O	-5.72	1.16	1.23
1	A	242	VAL	CA-CB	5.72	1.63	1.54
1	A	19	SER	CA-C	5.67	1.57	1.53
1	A	217	ALA	CA-CB	5.66	1.62	1.53
1	A	224	VAL	CA-CB	5.63	1.64	1.55
1	B	134	LEU	N-CA	5.62	1.52	1.46
1	B	21	VAL	CA-C	5.62	1.59	1.52
1	A	18	GLU	C-O	5.60	1.31	1.24
1	A	198	LYS	CA-CB	5.59	1.62	1.53
1	A	296	SER	CA-C	-5.57	1.46	1.52
1	B	4	ILE	CA-CB	5.56	1.61	1.54
1	B	282	PHE	CD2-CE2	5.55	1.55	1.38
1	A	69	TYR	CE1-CZ	5.55	1.51	1.38
1	A	299	GLY	N-CA	5.51	1.54	1.45
1	B	101	ARG	N-CA	5.49	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	GLY	N-CA	5.49	1.52	1.45
1	A	243	ASP	C-N	5.48	1.39	1.33
1	A	62	ALA	CA-CB	5.47	1.64	1.54
1	B	207	CYS	N-CA	5.46	1.52	1.46
1	B	179	ASP	N-CA	5.44	1.53	1.46
1	A	115	ALA	C-O	-5.44	1.17	1.23
1	A	116	GLY	CA-C	-5.44	1.46	1.52
1	B	190	ARG	C-O	5.41	1.30	1.24
1	B	227	LEU	N-CA	5.40	1.52	1.46
1	B	173	TYR	CE1-CZ	5.39	1.51	1.38
1	A	202	ILE	C-N	5.39	1.40	1.33
1	A	112	ARG	CG-CD	5.39	1.68	1.52
1	B	104	ASP	N-CA	-5.38	1.39	1.45
1	B	110	ALA	CA-CB	5.37	1.61	1.53
1	B	31	PHE	CD1-CE1	5.37	1.54	1.38
1	A	136	SER	C-O	5.37	1.29	1.23
1	A	240	LEU	C-O	5.36	1.29	1.24
1	B	200	GLU	N-CA	5.35	1.53	1.46
1	B	223	ARG	CZ-NH1	5.34	1.40	1.32
1	A	275	GLN	C-N	5.32	1.40	1.34
1	B	44	SER	C-O	-5.31	1.17	1.24
1	B	37	LYS	CA-C	5.30	1.59	1.53
1	B	284	ILE	N-CA	-5.30	1.40	1.46
1	B	48	GLN	CA-C	5.29	1.59	1.52
1	B	227	LEU	CB-CG	5.28	1.64	1.53
1	B	290	LYS	CG-CD	5.28	1.68	1.52
1	B	23	GLU	CA-C	5.27	1.59	1.52
1	A	103	ASN	CA-CB	5.27	1.62	1.52
1	B	52	VAL	CA-C	5.26	1.58	1.52
1	A	148	ASP	CA-C	5.25	1.60	1.53
1	B	293	ALA	CA-CB	-5.24	1.45	1.53
1	B	224	VAL	C-N	5.22	1.41	1.33
1	B	199	GLU	C-O	5.20	1.30	1.24
1	A	243	ASP	C-O	5.20	1.30	1.24
1	B	151	ASP	CG-OD1	5.18	1.35	1.25
1	A	14	CYS	CA-C	5.17	1.59	1.52
1	B	48	GLN	CD-OE1	5.16	1.33	1.23
1	A	206	MET	N-CA	-5.16	1.39	1.45
1	A	15	ARG	CD-NE	5.16	1.53	1.46
1	B	105	GLY	CA-C	5.15	1.56	1.51
1	B	131	GLN	CA-C	5.14	1.59	1.52
1	A	265	ASP	CB-CG	5.14	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	VAL	CA-CB	5.13	1.59	1.53
1	B	223	ARG	CB-CG	5.12	1.67	1.52
1	A	49	VAL	C-O	5.12	1.29	1.24
1	A	240	LEU	N-CA	5.12	1.53	1.45
1	B	230	VAL	C-O	-5.11	1.18	1.24
1	B	149	GLN	C-N	5.11	1.40	1.33
1	B	106	LYS	C-O	5.10	1.30	1.23
1	B	151	ASP	C-O	5.10	1.29	1.23
1	A	23	GLU	CA-C	5.10	1.59	1.53
1	B	204	ASP	C-O	5.09	1.30	1.24
1	B	236	GLN	C-O	5.08	1.30	1.23
1	A	143	VAL	N-CA	5.08	1.52	1.46
1	B	198	LYS	CA-C	5.07	1.60	1.52
1	A	137	LEU	CA-C	5.07	1.59	1.52
1	A	233	LYS	C-O	-5.07	1.17	1.23
1	A	202	ILE	N-CA	5.05	1.52	1.46
1	A	214	LEU	C-O	5.05	1.30	1.24
1	B	132	GLY	C-O	5.05	1.31	1.23
1	B	172	SER	CA-C	5.04	1.59	1.52
1	A	110	ALA	C-O	5.03	1.31	1.24
1	B	32	VAL	C-O	-5.03	1.18	1.23
1	B	173	TYR	CG-CD2	5.03	1.50	1.39
1	A	65	GLN	N-CA	-5.02	1.40	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	O-C-N	30.85	154.14	123.29
1	A	129	ARG	CA-C-N	-14.99	100.05	122.08
1	A	129	ARG	C-N-CA	-14.99	100.05	122.08
1	B	128	GLU	O-C-N	14.98	141.84	123.26
1	B	128	GLU	CA-C-N	14.59	150.27	123.27
1	B	128	GLU	C-N-CA	14.59	150.27	123.27
1	A	108	ASP	CB-CG-OD1	-11.12	92.83	118.40
1	B	149	GLN	OE1-CD-NE2	10.32	132.92	122.60
1	A	30	LEU	O-C-N	9.62	133.91	123.03
1	A	108	ASP	CB-CA-C	-9.03	92.38	110.17
1	B	202	ILE	CA-C-N	8.43	128.44	119.76
1	B	202	ILE	C-N-CA	8.43	128.44	119.76
1	A	15	ARG	N-CA-C	-8.43	102.05	111.07
1	A	129	ARG	CA-C-O	-8.37	112.33	121.28
1	A	130	HIS	N-CA-C	8.32	122.89	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ALA	CA-C-N	-8.25	114.11	122.69
1	A	115	ALA	C-N-CA	-8.25	114.11	122.69
1	A	19	SER	CA-C-O	-7.87	115.04	120.47
1	B	201	GLN	CB-CA-C	-7.76	105.47	116.34
1	B	107	VAL	CA-C-N	7.74	132.44	120.60
1	B	107	VAL	C-N-CA	7.74	132.44	120.60
1	B	108	ASP	CA-C-O	-7.14	112.62	120.69
1	B	198	LYS	CA-C-N	7.08	130.47	120.28
1	B	198	LYS	C-N-CA	7.08	130.47	120.28
1	A	108	ASP	CA-CB-CG	-7.05	105.55	112.60
1	A	146	TYR	CA-C-O	-6.91	112.57	120.24
1	A	108	ASP	CB-CG-OD2	6.83	134.11	118.40
1	A	124	PRO	N-CA-CB	6.83	110.42	103.25
1	B	124	PRO	N-CA-CB	6.78	110.37	103.25
1	A	99	ASN	N-CA-C	6.76	119.72	110.06
1	B	19	SER	CA-C-O	-6.68	115.86	120.47
1	B	243	ASP	N-CA-C	6.51	119.37	111.82
1	B	104	ASP	N-CA-C	6.51	119.67	110.50
1	A	128	GLU	CA-C-O	6.42	128.45	121.26
1	A	108	ASP	N-CA-C	6.36	123.87	109.81
1	B	144	LYS	N-CA-C	-6.08	99.74	109.96
1	A	55	ASP	N-CA-C	6.00	120.60	113.16
1	A	235	LEU	CD1-CG-CD2	-5.99	97.63	110.80
1	B	140	ASP	N-CA-C	5.97	120.30	113.19
1	B	238	VAL	N-CA-C	-5.95	99.06	107.75
1	A	41	ARG	CB-CA-C	5.92	118.88	110.24
1	A	202	ILE	CA-C-N	-5.91	113.87	120.14
1	A	202	ILE	C-N-CA	-5.91	113.87	120.14
1	B	151	ASP	N-CA-C	5.79	120.01	111.04
1	A	260	VAL	N-CA-C	5.68	116.30	108.12
1	A	223	ARG	CA-C-O	5.67	127.30	121.23
1	A	18	GLU	N-CA-C	5.66	116.84	108.86
1	A	162	HIS	N-CA-C	5.63	119.33	111.90
1	B	207	CYS	N-CA-C	-5.61	99.13	108.32
1	B	50	GLN	CB-CA-C	-5.60	100.04	109.50
1	A	126	VAL	CA-C-O	-5.55	113.84	120.78
1	A	206	MET	N-CA-CB	-5.54	101.22	111.52
1	B	201	GLN	CA-C-N	-5.45	118.67	122.59
1	B	201	GLN	C-N-CA	-5.45	118.67	122.59
1	A	30	LEU	CA-C-O	-5.44	115.02	121.66
1	A	264	ARG	CG-CD-NE	-5.43	100.05	112.00
1	B	39	VAL	CB-CA-C	5.40	117.61	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	MET	CA-CB-CG	-5.37	103.35	114.10
1	A	90	LEU	N-CA-C	5.36	118.29	111.69
1	B	129	ARG	N-CA-C	-5.29	102.33	109.95
1	A	177	ALA	N-CA-C	-5.27	101.06	109.23
1	A	273	LEU	CA-C-N	-5.19	114.50	122.60
1	A	273	LEU	C-N-CA	-5.19	114.50	122.60
1	A	171	LEU	N-CA-C	-5.18	106.98	113.15
1	B	34	ILE	N-CA-CB	5.14	114.46	110.45
1	A	88	VAL	CA-C-O	-5.08	115.09	120.48
1	B	83	LYS	N-CA-C	5.08	119.11	113.01
1	B	154	ASN	CA-C-N	-5.07	114.92	120.44
1	B	154	ASN	C-N-CA	-5.07	114.92	120.44
1	A	244	LYS	CB-CG-CD	-5.06	99.65	111.30
1	A	59	SER	N-CA-C	5.05	119.49	113.23
1	A	201	GLN	CB-CA-C	-5.01	109.33	116.34

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	THR	Peptide
1	A	124	PRO	Peptide
1	A	125	ALA	Peptide
1	A	127	LEU	Peptide
1	A	128	GLU	Peptide
1	B	123	ALA	Peptide
1	B	125	ALA	Peptide
1	B	126	VAL	Peptide
1	B	127	LEU	Peptide
1	B	128	GLU	Peptide

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	2303	0	2238	67	0
1	B	2303	0	2237	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	84	0	0	4	0
3	B	60	0	0	3	0
All	All	4752	0	4475	150	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 17.

All (150) 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:150:VAL:CA	1:B:150:VAL:CB	1.74	1.57
1:B:227:LEU:CD2	1:B:227:LEU:CG	1.76	1.55
1:A:294:PRO:CB	1:A:294:PRO:CG	1.79	1.43
1:B:195:LYS:NZ	1:A:127:LEU:N	1.67	1.34
1:B:195:LYS:NZ	1:A:127:LEU:H	0.84	1.31
1:B:195:LYS:HZ1	1:A:127:LEU:N	1.21	1.24
1:B:122:THR:O	1:B:125:ALA:HA	1.51	1.09
1:B:192:SER:HB3	1:A:126:VAL:HA	1.39	1.05
1:A:128:GLU:HA	1:A:129:ARG:HG3	1.38	1.03
1:A:108:ASP:HB3	1:A:110:ALA:H	1.28	0.99
1:B:192:SER:CB	1:A:126:VAL:HA	1.94	0.97
1:B:195:LYS:HZ2	1:A:127:LEU:H	0.94	0.91
1:B:140:ASP:OD1	1:B:142:HIS:ND1	2.04	0.89
1:B:195:LYS:HG3	1:A:125:ALA:HA	1.53	0.89
1:B:274:ARG:HA	1:B:274:ARG:HE	1.40	0.87
1:B:200:GLU:O	1:B:218:CYS:HB3	1.79	0.82
1:A:41:ARG:NH1	3:A:381:HOH:O	2.13	0.81
1:B:195:LYS:CG	1:A:125:ALA:HA	2.10	0.80
1:A:128:GLU:CA	1:A:129:ARG:HG3	2.13	0.78
1:B:195:LYS:HZ1	1:A:127:LEU:CA	1.97	0.77
1:B:194:TYR:CE1	1:B:227:LEU:HD22	2.19	0.77
1:B:195:LYS:CE	1:A:127:LEU:H	1.97	0.76
1:B:194:TYR:CD1	1:B:227:LEU:HD22	2.20	0.76
1:B:84:GLU:O	1:B:85:GLN:HB2	1.87	0.75
1:B:195:LYS:NZ	1:A:127:LEU:O	2.19	0.75
1:B:81:ASN:OD1	1:B:81:ASN:C	2.29	0.74
1:B:274:ARG:HA	1:B:274:ARG:NE	2.03	0.72
1:A:93:VAL:O	1:A:95:ASN:N	2.23	0.72
1:B:195:LYS:NZ	1:A:127:LEU:CA	2.51	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH2	1:A:182:LEU:O	2.20	0.71
1:B:195:LYS:HZ2	1:A:127:LEU:N	1.52	0.71
1:A:222:GLY:HA2	1:A:242:VAL:O	1.91	0.71
1:A:108:ASP:HB2	1:A:112:ARG:H	1.56	0.71
1:B:195:LYS:NZ	1:A:127:LEU:C	2.49	0.70
1:A:142:HIS:HB3	3:A:1:HOH:O	1.90	0.70
1:B:112:ARG:HG2	1:B:139:PRO:HD3	1.73	0.69
1:B:195:LYS:HG3	1:A:125:ALA:CA	2.21	0.69
1:A:140:ASP:CG	1:A:142:HIS:HD1	2.00	0.69
1:B:84:GLU:HG3	1:B:85:GLN:N	2.05	0.69
1:B:174:SER:HB2	1:B:195:LYS:HE2	1.75	0.68
1:B:58:VAL:HG13	1:B:73:ILE:HG12	1.75	0.68
1:B:227:LEU:CD2	1:B:227:LEU:HG	2.13	0.68
1:B:122:THR:C	1:B:124:PRO:HA	2.19	0.67
1:B:150:VAL:CA	1:B:150:VAL:HB	2.15	0.66
1:B:179:ASP:OD2	1:B:189:ASN:ND2	2.29	0.66
1:A:15:ARG:HB2	1:A:35:PRO:HG2	1.77	0.65
1:B:195:LYS:HZ1	1:A:127:LEU:H	0.67	0.64
1:B:39:VAL:CG2	1:B:58:VAL:HG11	2.26	0.64
1:B:122:THR:H	1:B:126:VAL:N	1.95	0.64
1:A:93:VAL:O	1:A:94:ASP:C	2.42	0.63
1:B:178:PHE:CE1	1:B:190:ARG:HB2	2.35	0.62
1:B:195:LYS:HE3	1:A:125:ALA:HA	1.80	0.62
1:B:84:GLU:O	1:B:85:GLN:CB	2.48	0.61
1:B:150:VAL:CB	1:B:150:VAL:C	2.72	0.60
1:B:150:VAL:CB	1:B:150:VAL:N	2.60	0.59
1:B:192:SER:HB3	1:A:126:VAL:CA	2.26	0.57
1:B:213:LYS:HD2	1:B:235:LEU:HD11	1.87	0.57
1:A:64:ARG:NH1	1:A:79:ALA:HB1	2.20	0.57
1:B:122:THR:C	1:B:125:ALA:HA	2.28	0.56
1:B:152:ILE:HB	1:B:170:SER:HB2	1.85	0.56
1:A:124:PRO:O	1:A:125:ALA:HB3	2.05	0.56
1:B:157:ASP:OD2	1:B:207:CYS:HA	2.06	0.56
1:A:179:ASP:O	1:A:187:ILE:HA	2.07	0.55
1:B:194:TYR:CE1	1:B:227:LEU:CD2	2.87	0.55
1:B:264:ARG:HG2	3:B:329:HOH:O	2.07	0.54
1:B:195:LYS:HZ3	1:A:127:LEU:C	2.14	0.54
1:B:195:LYS:CD	1:A:125:ALA:HA	2.37	0.54
1:B:250:PHE:CB	1:B:291:GLY:HA3	2.37	0.54
1:A:264:ARG:NH2	1:A:276:PRO:O	2.41	0.54
1:B:227:LEU:CD2	1:B:227:LEU:CD1	2.79	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:GLU:HG3	1:B:121:GLU:N	2.22	0.53
1:A:196:LEU:HD12	1:A:196:LEU:N	2.22	0.53
1:B:192:SER:HB2	1:A:126:VAL:HA	1.86	0.53
1:B:84:GLU:CG	1:B:85:GLN:N	2.70	0.53
1:B:105:GLY:HA2	1:B:114:PHE:O	2.09	0.53
1:A:200:GLU:O	1:A:218:CYS:HB3	2.09	0.53
1:B:119:ALA:HB2	1:B:131:GLN:HB2	1.91	0.53
1:A:124:PRO:O	1:A:125:ALA:CB	2.57	0.52
1:B:146:TYR:O	1:B:147:PHE:HB3	2.08	0.52
1:A:113:TYR:HB3	1:A:137:LEU:HB3	1.91	0.52
1:B:88:VAL:O	1:B:88:VAL:HG12	2.10	0.52
1:B:195:LYS:HG3	1:A:125:ALA:CB	2.40	0.51
1:B:195:LYS:CE	1:A:125:ALA:HA	2.39	0.51
1:B:204:ASP:CG	1:B:246:THR:O	2.53	0.51
1:B:264:ARG:CZ	1:B:272:LEU:HD22	2.40	0.51
1:B:221:GLY:O	1:B:222:GLY:C	2.52	0.51
1:B:82:TRP:HD1	1:B:83:LYS:HE3	1.75	0.51
1:A:77:PHE:HB3	1:A:137:LEU:HD22	1.93	0.51
1:B:206:MET:CG	1:B:207:CYS:N	2.73	0.51
1:B:56:ALA:HB3	1:B:73:ILE:HG22	1.93	0.50
1:B:250:PHE:HB2	1:B:291:GLY:HA3	1.92	0.50
1:B:130:HIS:O	1:B:149:GLN:HA	2.12	0.50
1:B:108:ASP:C	1:B:110:ALA:H	2.20	0.50
1:B:122:THR:O	1:B:124:PRO:N	2.45	0.49
1:A:15:ARG:HB3	1:A:265:ASP:OD1	2.12	0.49
1:A:15:ARG:HB3	1:A:265:ASP:CG	2.37	0.49
1:A:139:PRO:HG3	1:A:298:ALA:HB3	1.95	0.49
1:A:197:GLU:O	1:A:200:GLU:HB2	2.12	0.49
1:B:162:HIS:HB3	1:B:182:LEU:HD13	1.94	0.49
1:A:109:PRO:HB2	1:A:182:LEU:HD13	1.95	0.48
1:B:178:PHE:HB3	1:B:187:ILE:HB	1.95	0.48
1:B:150:VAL:CA	1:B:150:VAL:CG2	2.81	0.48
1:A:140:ASP:OD1	1:A:142:HIS:ND1	2.47	0.48
1:B:55:ASP:OD1	1:B:55:ASP:N	2.32	0.48
1:B:150:VAL:CA	1:B:150:VAL:CG1	2.85	0.48
1:B:81:ASN:OD1	1:B:81:ASN:O	2.32	0.47
1:A:197:GLU:OE1	1:A:234:ARG:NH1	2.43	0.47
1:B:250:PHE:CG	1:B:291:GLY:HA3	2.50	0.47
1:A:228:ASP:OD1	1:A:230:VAL:HG12	2.15	0.47
1:A:79:ALA:O	1:A:87:ALA:HA	2.15	0.47
1:B:69:TYR:HB2	1:B:80:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASP:HB3	1:B:110:ALA:H	1.80	0.46
1:B:220:ASN:HA	1:B:243:ASP:O	2.15	0.46
1:A:64:ARG:NH1	1:A:79:ALA:CB	2.78	0.46
1:B:145:LYS:HG2	1:B:146:TYR:H	1.80	0.46
1:A:219:TYR:C	1:A:221:GLY:H	2.22	0.46
1:B:122:THR:N	1:B:126:VAL:N	2.57	0.46
1:B:38:LYS:HE2	1:B:53:THR:OG1	2.16	0.46
1:B:201:GLN:HG3	1:B:220:ASN:C	2.41	0.46
3:B:328:HOH:O	1:A:130:HIS:CD2	2.69	0.45
1:A:213:LYS:HG3	1:A:235:LEU:CD1	2.46	0.45
1:A:128:GLU:C	1:A:129:ARG:HG3	2.42	0.45
1:A:47:LYS:HB3	3:A:374:HOH:O	2.18	0.44
1:A:64:ARG:NE	1:A:299:GLY:O	2.42	0.44
1:B:209:ASP:OD1	1:B:209:ASP:C	2.61	0.44
1:B:195:LYS:HZ1	1:A:127:LEU:C	2.18	0.43
1:B:226:ARG:HG2	1:B:227:LEU:N	2.32	0.43
1:A:76:LYS:HD2	3:A:314:HOH:O	2.18	0.43
1:B:10:LEU:HA	1:B:11:PRO:HD3	1.74	0.43
1:B:173:TYR:CD2	1:B:173:TYR:N	2.87	0.43
1:A:103:ASN:HB3	1:A:153:SER:O	2.19	0.43
1:B:244:LYS:HE2	1:B:267:MET:HE3	2.00	0.43
1:B:15:ARG:HB2	1:B:35:PRO:HG2	2.01	0.42
1:B:169:ASP:C	1:B:169:ASP:OD1	2.63	0.42
1:B:180:TYR:HB2	1:B:187:ILE:HG22	2.02	0.42
1:A:152:ILE:HB	1:A:170:SER:HB2	2.02	0.42
1:B:103:ASN:HB3	1:B:153:SER:O	2.19	0.42
1:B:39:VAL:HG22	1:B:58:VAL:HG11	2.01	0.41
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.80	0.41
1:B:226:ARG:HD3	1:B:235:LEU:HD12	2.02	0.41
1:B:122:THR:C	1:B:124:PRO:CA	2.93	0.41
1:B:156:LEU:HA	1:B:166:TYR:O	2.20	0.41
1:B:264:ARG:HH21	1:B:278:ALA:HB3	1.84	0.41
1:B:264:ARG:CG	3:B:329:HOH:O	2.68	0.41
1:B:208:ILE:HG13	1:B:213:LYS:O	2.20	0.41
1:B:264:ARG:HE	1:B:264:ARG:HB2	1.39	0.40
1:A:220:ASN:HD21	1:A:244:LYS:NZ	2.20	0.40
1:B:105:GLY:CA	1:B:114:PHE:O	2.69	0.40
1:B:178:PHE:CD1	1:B:190:ARG:HB2	2.57	0.40
1:A:64:ARG:HH11	1:A:79:ALA:HB1	1.86	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	295/297 (99%)	269 (91%)	21 (7%)	5 (2%)	7	2
1	B	295/297 (99%)	262 (89%)	25 (8%)	8 (3%)	4	0
All	All	590/594 (99%)	531 (90%)	46 (8%)	13 (2%)	5	0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	GLN
1	B	123	ALA
1	B	124	PRO
1	B	126	VAL
1	B	130	HIS
1	B	173	TYR
1	A	94	ASP
1	A	124	PRO
1	B	99	ASN
1	A	127	LEU
1	A	108	ASP
1	B	127	LEU
1	A	125	ALA

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	246/252 (98%)	231 (94%)	15 (6%)	17	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	246/252 (98%)	224 (91%)	22 (9%)	9	1
All	All	492/504 (98%)	455 (92%)	37 (8%)	12	3

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	ILE
1	B	58	VAL
1	B	81	ASN
1	B	83	LYS
1	B	84	GLU
1	B	86	SER
1	B	98	LYS
1	B	99	ASN
1	B	129	ARG
1	B	156	LEU
1	B	180	TYR
1	B	183	GLN
1	B	198	LYS
1	B	200	GLU
1	B	230	VAL
1	B	231	THR
1	B	253	LYS
1	B	264	ARG
1	B	267	MET
1	B	270	GLU
1	B	274	ARG
1	B	289	VAL
1	A	3	SER
1	A	49	VAL
1	A	80	LEU
1	A	98	LYS
1	A	144	LYS
1	A	153	SER
1	A	178	PHE
1	A	183	GLN
1	A	195	LYS
1	A	198	LYS
1	A	199	GLU
1	A	227	LEU
1	A	240	LEU
1	A	253	LYS

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Mol	Chain	Res	Type
1	A	274	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	99	ASN
1	B	149	GLN
1	A	99	ASN
1	A	100	ASN
1	A	220	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	128:GLU	C	129:ARG	N	1.62

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	297/297 (100%)	0.63	13 (4%)	39 43	20, 41, 57, 65	0
1	B	297/297 (100%)	0.91	31 (10%)	11 15	20, 50, 73, 86	0
All	All	594/594 (100%)	0.77	44 (7%)	20 24	20, 45, 65, 86	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	17.0
1	A	126	VAL	15.0
1	A	125	ALA	12.0
1	B	123	ALA	10.7
1	B	125	ALA	8.4
1	A	124	PRO	7.8
1	B	127	LEU	7.6
1	A	123	ALA	7.6
1	B	126	VAL	7.6
1	A	122	THR	7.2
1	B	124	PRO	7.0
1	A	128	GLU	6.0
1	B	122	THR	6.0
1	A	121	GLU	4.8
1	B	121	GLU	4.7
1	B	128	GLU	4.7
1	B	272	LEU	3.2
1	B	269	PRO	2.9
1	B	177	ALA	2.8
1	B	194	TYR	2.8
1	B	152	ILE	2.7
1	B	229	PRO	2.7
1	B	80	LEU	2.7
1	B	273	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	93	VAL	2.7
1	A	68	GLY	2.5
1	B	88	VAL	2.5
1	B	185	GLY	2.3
1	A	266	GLY	2.3
1	B	133	ALA	2.3
1	B	276	PRO	2.3
1	B	242	VAL	2.3
1	B	84	GLU	2.3
1	B	225	ILE	2.3
1	A	129	ARG	2.3
1	B	230	VAL	2.3
1	B	147	PHE	2.2
1	A	96	ASP	2.2
1	B	45	PHE	2.2
1	B	82	TRP	2.2
1	B	178	PHE	2.1
1	B	274	ARG	2.1
1	B	187	ILE	2.0
1	B	146	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	300	1/1	0.96	0.07	61,61,61,61	0
2	ZN	B	300	1/1	0.98	0.04	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.