Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:56 pm GMT

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PDB ID	:	3G4H
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)

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	Percentile Ranks	Value
Rfree		0.308
Clashscore		16
Ramachandran outliers		2.2%
Sidechain outliers		6.9%
RSRZ outliers		22.4%

Worse → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
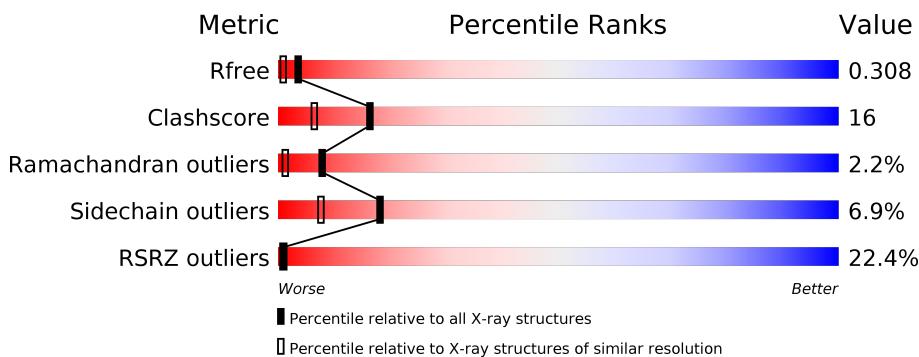
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6276 (1.94-1.90)
Clashscore	112137	7025 (1.94-1.90)
Ramachandran outliers	110173	6947 (1.94-1.90)
Sidechain outliers	110143	6948 (1.94-1.90)
RSRZ outliers	101464	6332 (1.94-1.90)

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	297	18% / 60% 33% 6% •
1	B	297	27% / 57% 32% 9% •
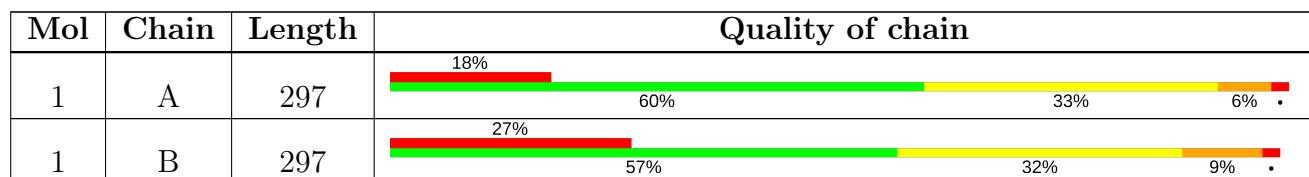
2 Entry composition ⓘ

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 (three-letter code: 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	A	84	Total	O	0	0
			84	84		
3	B	60	Total	O	0	0
			60	60		

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: Regucalcin
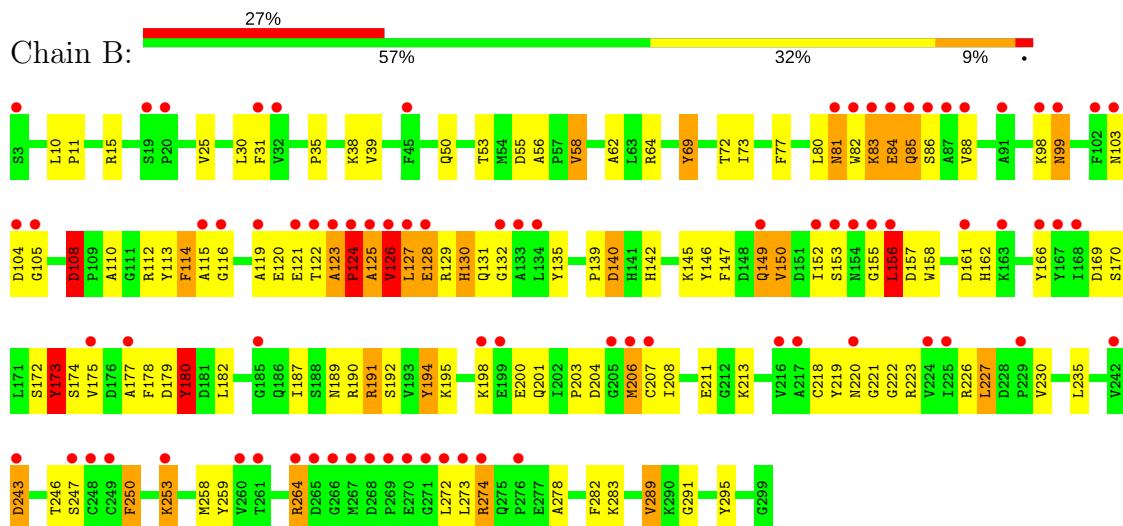
- Molecule 1: Regucalcin
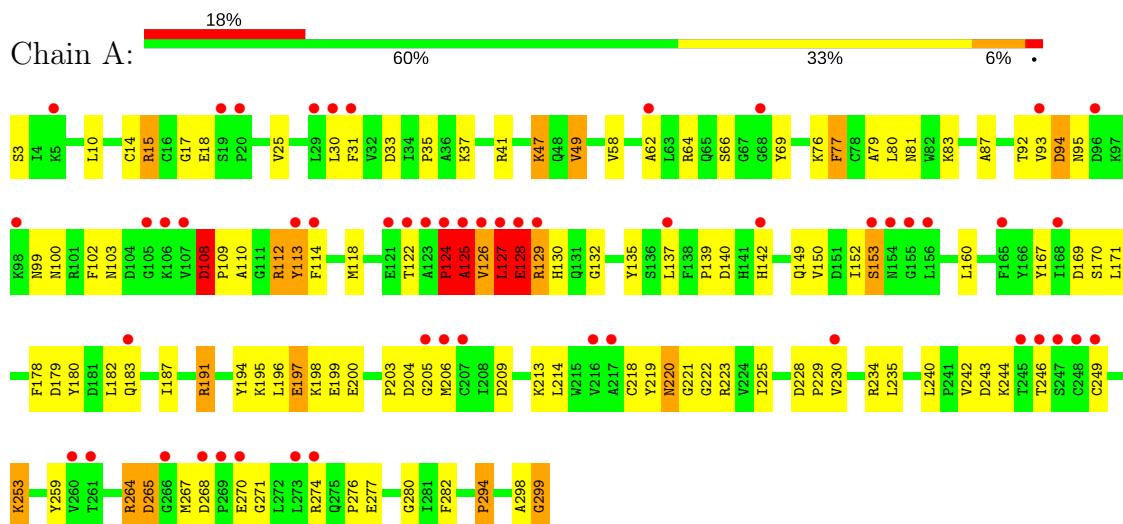
4 Data and refinement statistics ⓘ

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 26.01 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.2 (84.52-1.92) 99.3 (26.01-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.253 0.239 , 0.308	Depositor DCC
R_{free} test set	2148 reflections (5.29%)	DCC
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 , 43.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.96	57/2353 (2.4%)	1.65	35/3185 (1.1%)
1	B	1.96	55/2353 (2.3%)	1.41	20/3185 (0.6%)
All	All	1.96	112/4706 (2.4%)	1.54	55/6370 (0.9%)

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 (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	180	TYR	CD1-CE1	12.91	1.58	1.39
1	A	128	GLU	C-N	12.16	1.62	1.34
1	A	69	TYR	CE1-CZ	10.01	1.51	1.38
1	A	108	ASP	CB-CG	-9.89	1.30	1.51
1	B	173	TYR	CE1-CZ	9.72	1.51	1.38
1	B	243	ASP	C-O	9.66	1.41	1.23
1	A	66	SER	CB-OG	9.64	1.54	1.42
1	B	155	GLY	N-CA	9.48	1.60	1.46
1	B	150	VAL	CA-CB	9.39	1.74	1.54
1	A	150	VAL	CA-CB	9.31	1.74	1.54
1	B	180	TYR	CD2-CE2	9.29	1.53	1.39
1	B	247	SER	CB-OG	9.28	1.54	1.42
1	B	135	TYR	CD1-CE1	9.03	1.52	1.39
1	B	173	TYR	CD1-CE1	8.73	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	C-N	8.57	1.53	1.34
1	A	205	GLY	N-CA	8.56	1.58	1.46
1	B	177	ALA	C-O	8.47	1.39	1.23
1	A	69	TYR	CE2-CZ	8.43	1.49	1.38
1	B	173	TYR	CG-CD2	8.27	1.50	1.39
1	B	69	TYR	CD1-CE1	8.24	1.51	1.39
1	A	102	PHE	CE1-CZ	8.16	1.52	1.37
1	B	282	PHE	CD2-CE2	8.03	1.55	1.39
1	A	127	LEU	C-N	7.86	1.52	1.34
1	B	180	TYR	CE2-CZ	7.81	1.48	1.38
1	B	31	PHE	CD1-CE1	7.75	1.54	1.39
1	B	108	ASP	CB-CG	-7.66	1.35	1.51
1	A	18	GLU	CD-OE1	7.55	1.33	1.25
1	A	14	CYS	CB-SG	7.48	1.95	1.82
1	A	280	GLY	N-CA	7.44	1.57	1.46
1	B	104	ASP	CB-CG	7.41	1.67	1.51
1	B	173	TYR	CD2-CE2	7.26	1.50	1.39
1	B	135	TYR	CE2-CZ	7.23	1.48	1.38
1	B	203	PRO	C-O	7.10	1.37	1.23
1	B	223	ARG	NE-CZ	7.03	1.42	1.33
1	A	15	ARG	CB-CG	7.01	1.71	1.52
1	A	114	PHE	CE1-CZ	6.87	1.50	1.37
1	A	259	TYR	CD2-CE2	6.83	1.49	1.39
1	B	206	MET	CG-SD	6.81	1.98	1.81
1	B	175	VAL	CA-CB	6.77	1.69	1.54
1	A	194	TYR	CG-CD1	6.74	1.48	1.39
1	A	112	ARG	CG-CD	6.66	1.68	1.51
1	B	227	LEU	CG-CD2	6.65	1.76	1.51
1	B	149	GLN	CD-OE1	6.58	1.38	1.24
1	B	135	TYR	CD2-CE2	6.48	1.49	1.39
1	A	259	TYR	CD1-CE1	6.42	1.49	1.39
1	B	158	TRP	CG-CD1	6.38	1.45	1.36
1	A	83	LYS	C-O	6.35	1.35	1.23
1	A	282	PHE	CD2-CE2	6.35	1.51	1.39
1	A	37	LYS	CD-CE	6.28	1.67	1.51
1	B	250	PHE	CE1-CZ	6.28	1.49	1.37
1	A	265	ASP	CB-CG	6.26	1.64	1.51
1	B	180	TYR	CG-CD1	6.23	1.47	1.39
1	A	249	CYS	CB-SG	6.05	1.92	1.82
1	A	132	GLY	C-O	6.03	1.33	1.23
1	A	49	VAL	CA-CB	6.02	1.67	1.54
1	B	219	TYR	CE2-CZ	5.97	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	PHE	CD1-CE1	5.92	1.51	1.39
1	A	58	VAL	CB-CG2	-5.88	1.40	1.52
1	A	197	GLU	C-O	5.86	1.34	1.23
1	A	229	PRO	CA-C	5.84	1.64	1.52
1	A	294	PRO	CB-CG	5.83	1.79	1.50
1	B	77	PHE	CE1-CZ	5.80	1.48	1.37
1	B	194	TYR	CD1-CE1	5.79	1.48	1.39
1	A	77	PHE	CD1-CE1	5.77	1.50	1.39
1	B	114	PHE	C-O	5.74	1.34	1.23
1	A	135	TYR	CZ-OH	5.74	1.47	1.37
1	A	102	PHE	CG-CD1	5.74	1.47	1.38
1	A	203	PRO	N-CA	5.70	1.56	1.47
1	B	115	ALA	CA-CB	5.70	1.64	1.52
1	A	100	ASN	C-O	5.69	1.34	1.23
1	A	62	ALA	CA-CB	5.67	1.64	1.52
1	B	223	ARG	CB-CG	5.65	1.67	1.52
1	A	271	GLY	N-CA	5.63	1.54	1.46
1	A	180	TYR	CD1-CE1	5.62	1.47	1.39
1	B	62	ALA	CA-CB	5.62	1.64	1.52
1	A	69	TYR	CG-CD2	5.61	1.46	1.39
1	A	220	ASN	CG-ND2	5.61	1.46	1.32
1	B	113	TYR	CD1-CE1	5.57	1.47	1.39
1	A	180	TYR	CB-CG	5.56	1.59	1.51
1	A	299	GLY	N-CA	5.54	1.54	1.46
1	A	31	PHE	CG-CD2	5.52	1.47	1.38
1	B	223	ARG	CZ-NH1	5.52	1.40	1.33
1	A	47	LYS	CG-CD	5.52	1.71	1.52
1	B	295	TYR	CD2-CE2	5.52	1.47	1.39
1	B	149	GLN	CD-NE2	5.50	1.46	1.32
1	B	161	ASP	CB-CG	5.49	1.63	1.51
1	A	246	THR	C-N	5.44	1.46	1.34
1	B	295	TYR	CE2-CZ	5.42	1.45	1.38
1	A	17	GLY	N-CA	5.39	1.54	1.46
1	A	225	ILE	CA-CB	5.36	1.67	1.54
1	B	253	LYS	CG-CD	5.35	1.70	1.52
1	A	149	GLN	N-CA	5.35	1.57	1.46
1	A	66	SER	C-O	-5.32	1.13	1.23
1	A	253	LYS	CD-CE	5.32	1.64	1.51
1	A	169	ASP	C-O	5.31	1.33	1.23
1	B	116	GLY	N-CA	-5.28	1.38	1.46
1	B	194	TYR	CG-CD1	5.23	1.46	1.39
1	A	114	PHE	CG-CD1	5.22	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	GLU	CD-OE1	5.21	1.31	1.25
1	A	81	ASN	CB-CG	5.14	1.62	1.51
1	B	180	TYR	CG-CD2	5.13	1.45	1.39
1	B	211	GLU	CB-CG	5.12	1.61	1.52
1	B	77	PHE	CE2-CZ	5.10	1.47	1.37
1	A	299	GLY	C-O	5.08	1.31	1.23
1	B	25	VAL	CB-CG1	5.06	1.63	1.52
1	A	92	THR	N-CA	5.05	1.56	1.46
1	B	140	ASP	CG-OD2	5.04	1.36	1.25
1	A	270	GLU	CD-OE1	5.03	1.31	1.25
1	B	259	TYR	CE2-CZ	5.02	1.45	1.38
1	B	132	GLY	C-O	5.01	1.31	1.23
1	B	250	PHE	CG-CD2	5.00	1.46	1.38
1	A	126	VAL	C-O	5.00	1.32	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	ASP	CB-CG-OD1	-28.30	92.83	118.30
1	A	129	ARG	O-C-N	19.65	154.14	122.70
1	A	108	ASP	CB-CG-OD2	17.57	134.11	118.30
1	A	129	ARG	CA-C-N	-12.39	89.95	117.20
1	B	128	GLU	O-C-N	11.96	141.84	122.70
1	B	128	GLU	CA-C-N	-11.74	91.37	117.20
1	B	128	GLU	C-N-CA	11.43	150.27	121.70
1	B	108	ASP	CB-CG-OD1	-10.80	108.58	118.30
1	A	33	ASP	CB-CG-OD2	9.33	126.69	118.30
1	B	104	ASP	CB-CG-OD1	9.17	126.55	118.30
1	A	264	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	265	ASP	CB-CG-OD1	9.10	126.49	118.30
1	A	108	ASP	CB-CA-C	-9.01	92.38	110.40
1	A	209	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	129	ARG	C-N-CA	-8.66	100.05	121.70
1	B	30	LEU	CB-CG-CD1	-8.62	96.35	111.00
1	A	223	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	B	161	ASP	CB-CG-OD1	8.55	125.99	118.30
1	A	268	ASP	CB-CG-OD1	8.26	125.73	118.30
1	A	77	PHE	CB-CG-CD1	8.16	126.51	120.80
1	A	33	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	A	30	LEU	O-C-N	7.00	133.91	122.70
1	B	104	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	167	TYR	CB-CG-CD1	-6.69	116.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	273	LEU	CA-CB-CG	6.64	130.57	115.30
1	A	167	TYR	CB-CG-CD2	6.37	124.82	121.00
1	B	72	THR	CA-CB-CG2	-6.24	103.67	112.40
1	B	156	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	69	TYR	CZ-CE2-CD2	-5.98	114.42	119.80
1	A	124	PRO	N-CA-CB	5.93	110.42	103.30
1	B	124	PRO	N-CA-CB	5.89	110.37	103.30
1	B	258	MET	CA-CB-CG	-5.85	103.35	113.30
1	B	283	LYS	CD-CE-NZ	-5.72	98.54	111.70
1	A	264	ARG	CG-CD-NE	-5.59	100.05	111.80
1	B	169	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	108	ASP	CB-CG-OD2	5.47	123.23	118.30
1	A	214	LEU	CB-CG-CD1	-5.43	101.77	111.00
1	A	160	LEU	CB-CG-CD1	-5.39	101.84	111.00
1	B	191	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	171	LEU	CB-CG-CD1	5.31	120.03	111.00
1	A	204	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	A	191	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	A	206	MET	N-CA-CB	-5.21	101.22	110.60
1	B	50	GLN	CB-CA-C	-5.18	100.04	110.40
1	A	267	MET	CA-CB-CG	-5.16	104.52	113.30
1	B	289	VAL	CG1-CB-CG2	5.12	119.10	110.90
1	B	64	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	112	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	10	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	243	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	108	ASP	OD1-CG-OD2	5.07	132.94	123.30
1	A	25	VAL	CG1-CB-CG2	5.06	118.99	110.90
1	A	118	MET	CG-SD-CE	5.04	108.27	100.20
1	A	206	MET	CG-SD-CE	5.04	108.26	100.20
1	A	58	VAL	CG1-CB-CG2	5.02	118.93	110.90

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

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Mol	Chain	Res	Type	Group
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	66	0
1	B	2303	0	2237	102	0
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	145	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 (145) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:112:ARG:NH2	1:A:182:LEU:O	2.20	0.71
1:B:195:LYS:NZ	1:A:127:LEU:CA	2.51	0.71
1:A:222:GLY:HA2	1:A:242:VAL:O	1.91	0.71
1:B:195:LYS:HZ2	1:A:127:LEU:N	1.52	0.71
1:A:108:ASP:HB2	1:A:112:ARG:H	1.56	0.71
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:B:84:GLU:HG3	1:B:85:GLN:N	2.05	0.69
1:B:81:ASN:OD1	1:B:81:ASN:C	2.29	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:HG	1:B:227:LEU:CD2	2.13	0.68
1:B:150:VAL:HB	1:B:150:VAL:CA	2.15	0.66
1:B:195:LYS:NZ	1:A:127:LEU:C	2.49	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:A:140:ASP:CG	1:A:142:HIS:HD1	2.00	0.64
1:B:122:THR:H	1:B:126:VAL:N	1.95	0.64
1:B:122:THR:C	1:B:124:PRO:HA	2.19	0.62
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:N	1:B:150:VAL:CB	2.60	0.59
1:A:93:VAL:O	1:A:94:ASP:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:SER:HB3	1:A:126:VAL:CA	2.26	0.57
1:A:64:ARG:NH1	1:A:79:ALA:HB1	2.20	0.57
1:B:213:LYS:HD2	1:B:235:LEU:HD11	1.87	0.57
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: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:120:GLU:HG3	1:B:121:GLU:N	2.22	0.54
1:B:227:LEU:CD2	1:B:227:LEU:CD1	2.79	0.53
1:A:196:LEU:N	1:A:196:LEU:HD12	2.22	0.53
1:B:192:SER:HB2	1:A:126:VAL:HA	1.86	0.53
1:B:105:GLY:HA2	1:B:114:PHE:O	2.09	0.53
1:B:84:GLU:CG	1:B:85:GLN:N	2.70	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:122:THR:N	1:B:126:VAL:N	2.57	0.52
1:B:88:VAL:O	1:B:88:VAL:HG12	2.10	0.52
1:B:122:THR:C	1:B:125:ALA:HA	2.28	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:264:ARG:CZ	1:B:272:LEU:HD22	2.40	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: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: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:150:VAL:C	1:B:150:VAL:CB	2.72	0.49
1:B:162:HIS:HB3	1:B:182:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:81:ASN:OD1	2.32	0.47
1:A:197:GLU:OE1	1:A:234:ARG:NH1	2.43	0.47
1:A:228:ASP:OD1	1:A:230:VAL:HG12	2.15	0.47
1:B:250:PHE:CG	1:B:291:GLY:HA3	2.50	0.47
1:A:79:ALA:O	1:A:87:ALA:HA	2.15	0.47
1:B:221:GLY:O	1:B:222:GLY:C	2.52	0.47
1:B:69:TYR:HB2	1:B:80:LEU:HB3	1.97	0.47
1:A:64:ARG:NH1	1:A:79:ALA:CB	2.78	0.46
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:B:204:ASP:CG	1:B:246:THR:O	2.53	0.46
1:B:145:LYS:HG2	1:B:146:TYR:H	1.80	0.46
1:B:38:LYS:HE2	1:B:53:THR:OG1	2.16	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:B:108:ASP:C	1:B:110:ALA:H	2.20	0.45
1:A:15:ARG:HB3	1:A:265:ASP:CG	2.37	0.44
1:A:64:ARG:NE	1:A:299:GLY:O	2.42	0.44
1:A:47:LYS:HB3	3:A:374:HOH:O	2.18	0.44
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:15:ARG:HB2	1:B:35:PRO:HG2	2.01	0.42
1:A:152:ILE:HB	1:A:170:SER:HB2	2.02	0.42
1:B:180:TYR:HB2	1:B:187:ILE:HG22	2.02	0.42
1:B:103:ASN:HB3	1:B:153:SER:O	2.19	0.42
1:A:219:TYR:C	1:A:221:GLY:H	2.22	0.42
1:B:195:LYS:HZ3	1:A:127:LEU:C	2.14	0.41
1:B:226:ARG:HD3	1:B:235:LEU:HD12	2.02	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLN:HG3	1:B:220:ASN:C	2.41	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:A:128:GLU:C	1:A:129:ARG:HG3	2.42	0.40
1:A:64:ARG:HH11	1:A:79:ALA:HB1	1.86	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

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	295/297 (99%)	269 (91%)	21 (7%)	5 (2%)	11	2
1	B	295/297 (99%)	262 (89%)	25 (8%)	8 (3%)	6	1
All	All	590/594 (99%)	531 (90%)	46 (8%)	13 (2%)	8	1

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

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Mol	Chain	Res	Type
1	A	127	LEU
1	A	108	ASP
1	B	127	LEU
1	A	125	ALA

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	246/252 (98%)	231 (94%)	15 (6%)	22	10
1	B	246/252 (98%)	227 (92%)	19 (8%)	15	6
All	All	492/504 (98%)	458 (93%)	34 (7%)	18	7

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	108	ASP
1	B	129	ARG
1	B	156	LEU
1	B	172	SER
1	B	180	TYR
1	B	191	ARG
1	B	198	LYS
1	B	230	VAL
1	B	253	LYS
1	B	264	ARG
1	B	274	ARG
1	B	289	VAL

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Mol	Chain	Res	Type
1	A	3	SER
1	A	49	VAL
1	A	80	LEU
1	A	99	ASN
1	A	113	TYR
1	A	153	SER
1	A	178	PHE
1	A	183	GLN
1	A	191	ARG
1	A	195	LYS
1	A	198	LYS
1	A	199	GLU
1	A	240	LEU
1	A	253	LYS
1	A	274	ARG

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

Mol	Chain	Res	Type
1	B	99	ASN
1	B	149	GLN
1	B	275	GLN
1	A	99	ASN
1	A	149	GLN
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 carbohydrates 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 ⓘ

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, 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%)	1.10	53 (17%)	2	2	20, 41, 57, 65	0
1	B	297/297 (100%)	1.53	80 (26%)	1	0	20, 50, 73, 86	0
All	All	594/594 (100%)	1.31	133 (22%)	1	1	20, 45, 65, 86	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	127	LEU	20.9
1	A	126	VAL	17.8
1	A	125	ALA	14.6
1	B	123	ALA	13.5
1	B	126	VAL	12.2
1	B	127	LEU	11.3
1	B	125	ALA	10.7
1	A	123	ALA	10.3
1	B	272	LEU	9.9
1	B	124	PRO	9.0
1	A	124	PRO	8.9
1	A	122	THR	8.8
1	B	122	THR	8.7
1	B	269	PRO	7.9
1	B	267	MET	7.4
1	B	276	PRO	7.2
1	B	273	LEU	6.9
1	B	156	LEU	6.7
1	A	121	GLU	6.1
1	B	86	SER	6.1
1	B	121	GLU	6.0
1	A	266	GLY	5.9
1	B	274	ARG	5.9
1	A	128	GLU	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLY	5.7
1	B	266	GLY	5.6
1	A	156	LEU	5.5
1	B	168	ILE	5.4
1	B	128	GLU	4.7
1	B	155	GLY	4.6
1	B	84	GLU	4.6
1	B	270	GLU	4.5
1	B	206	MET	4.4
1	A	107	VAL	4.4
1	A	155	GLY	4.2
1	B	247	SER	4.0
1	A	217	ALA	3.9
1	B	81	ASN	3.8
1	B	98	LYS	3.8
1	B	260	VAL	3.8
1	A	168	ILE	3.8
1	B	265	ASP	3.7
1	B	248	CYS	3.7
1	B	167	TYR	3.7
1	A	216	VAL	3.5
1	B	45	PHE	3.4
1	A	247	SER	3.3
1	A	98	LYS	3.3
1	B	82	TRP	3.3
1	A	96	ASP	3.3
1	B	99	ASN	3.3
1	B	185	GLY	3.2
1	B	154	ASN	3.2
1	B	205	GLY	3.2
1	B	104	ASP	3.2
1	A	230	VAL	3.1
1	B	220	ASN	3.1
1	B	91	ALA	3.1
1	A	246	THR	3.0
1	A	114	PHE	3.0
1	B	207	CYS	3.0
1	B	20	PRO	3.0
1	B	249	CYS	2.9
1	A	20	PRO	2.9
1	A	274	ARG	2.9
1	B	149	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	2.9
1	B	217	ALA	2.9
1	B	115	ALA	2.9
1	A	273	LEU	2.8
1	A	19	SER	2.8
1	B	105	GLY	2.8
1	B	85	GLN	2.8
1	B	268	ASP	2.7
1	B	225	ILE	2.7
1	B	87	ALA	2.7
1	A	62	ALA	2.7
1	B	134	LEU	2.7
1	A	248	CYS	2.7
1	A	5	LYS	2.6
1	B	224	VAL	2.6
1	A	207	CYS	2.6
1	A	249	CYS	2.6
1	B	116	GLY	2.6
1	A	165	PHE	2.6
1	B	19	SER	2.6
1	B	264	ARG	2.6
1	B	198	LYS	2.6
1	A	270	GLU	2.6
1	B	152	ILE	2.6
1	B	177	ALA	2.5
1	B	88	VAL	2.5
1	A	245	THR	2.5
1	B	229	PRO	2.4
1	A	269	PRO	2.4
1	B	133	ALA	2.4
1	A	154	ASN	2.4
1	B	83	LYS	2.4
1	B	199	GLU	2.4
1	A	113	TYR	2.3
1	B	132	GLY	2.3
1	A	142	HIS	2.3
1	B	216	VAL	2.3
1	B	242	VAL	2.3
1	A	260	VAL	2.3
1	A	30	LEU	2.3
1	B	163	LYS	2.3
1	A	29	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	103	ASN	2.2
1	B	119	ALA	2.2
1	B	261	THR	2.2
1	B	161	ASP	2.2
1	B	243	ASP	2.2
1	A	206	MET	2.2
1	A	68	GLY	2.2
1	A	183	GLN	2.2
1	B	3	SER	2.1
1	B	166	TYR	2.1
1	A	106	LYS	2.1
1	A	137	LEU	2.1
1	B	153	SER	2.1
1	A	105	GLY	2.1
1	A	31	PHE	2.1
1	A	261	THR	2.1
1	B	253	LYS	2.1
1	A	153	SER	2.1
1	A	268	ASP	2.1
1	A	93	VAL	2.1
1	B	31	PHE	2.0
1	B	175	VAL	2.0
1	B	32	VAL	2.0
1	B	102	PHE	2.0
1	A	129	ARG	2.0

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	300	1/1	0.93	0.18	-1.55	61,61,61,61	0
2	ZN	B	300	1/1	0.96	0.12	-2.51	80,80,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.