



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:22 PM UTC

PDB ID : 1PU0 / pdb_00001pu0
Title : Structure of Human Cu,Zn Superoxide Dismutase
Authors : DiDonato, M.; Craig, L.; Huff, M.E.; Thayer, M.M.; Cardoso, R.M.F.; Kassmann, C.J.; Lo, T.P.; Bruns, C.K.; Powers, E.T.; Kelly, J.W.; Getzoff, E.D.; Tainer, J.A.
Deposited on : 2003-06-23
Resolution : 1.70 Å(reported)

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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

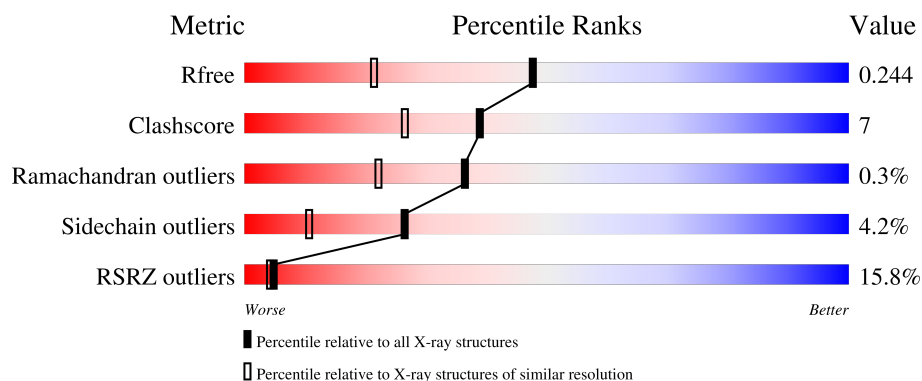
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	153	6% 92% 8%
1	B	153	6% 90% 8%
1	C	153	53% 70% 30%
1	D	153	6% 88% 11%
1	E	153	5% 90% 10%

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Mol	Chain	Length	Quality of chain
1	F	153	8% 90% 10%
1	G	153	34% 76% 23%
1	H	153	8% 87% 12%
1	I	153	22% 82% 18%
1	J	153	10% 86% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12222 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 Superoxide dismutase [Cu-Zn].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	B	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	C	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	D	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	E	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	F	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	G	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	H	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	I	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			
1	J	153	Total	C	N	O	S	0	2	0
			1114	681	203	224	6			

- Molecule 2 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		
2	B	1	Total	Cu	0	0
			1	1		
2	C	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		

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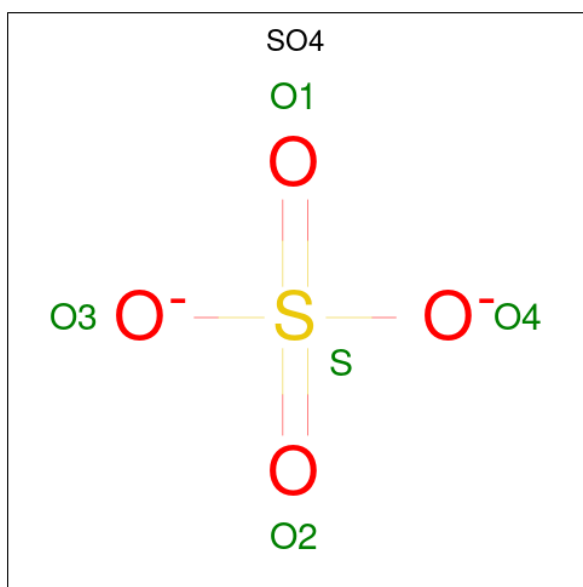
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		
2	G	1	Total	Cu	0	0
			1	1		
2	H	1	Total	Cu	0	0
			1	1		
2	I	1	Total	Cu	0	0
			1	1		
2	J	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	I	1	Total	Zn	0	0
			1	1		
3	J	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	131	Total	O	0	0
			131	131		
5	B	141	Total	O	0	0
			141	141		
5	C	57	Total	O	0	0
			57	57		
5	D	133	Total	O	0	0
			133	133		
5	E	133	Total	O	0	0
			133	133		
5	F	126	Total	O	0	0
			126	126		
5	G	55	Total	O	0	0
			55	55		
5	H	107	Total	O	0	0
			107	107		
5	I	60	Total	O	0	0
			60	60		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	104	Total 104	O 104	0	0

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.

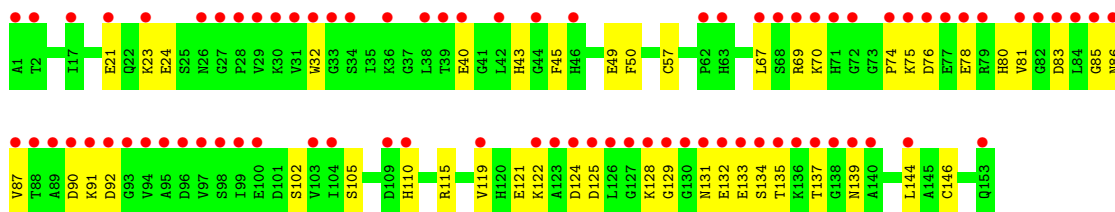
- Molecule 1: Superoxide dismutase [Cu-Zn]



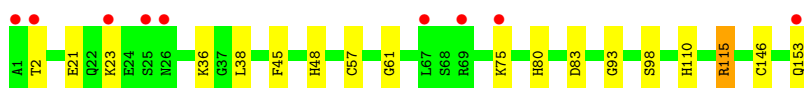
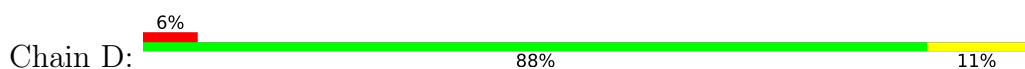
- Molecule 1: Superoxide dismutase [Cu-Zn]



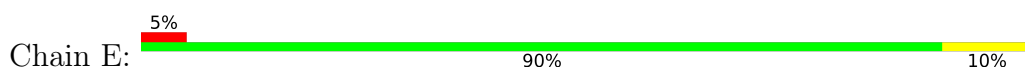
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]

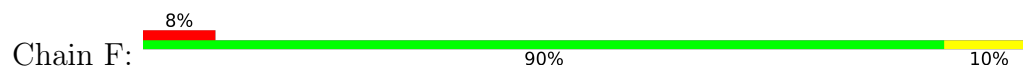


- Molecule 1: Superoxide dismutase [Cu-Zn]

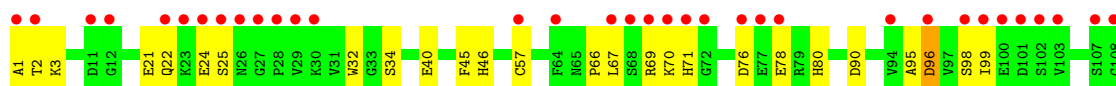
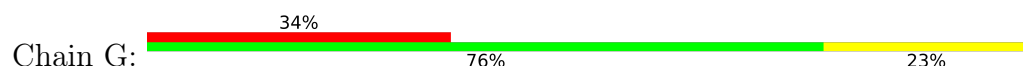




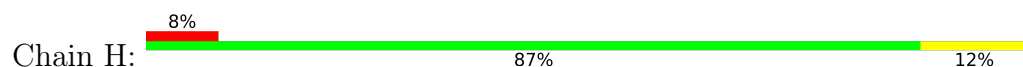
- Molecule 1: Superoxide dismutase [Cu-Zn]



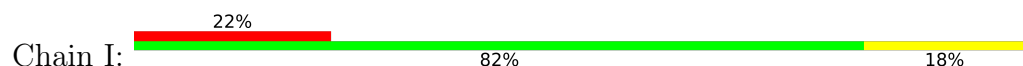
- Molecule 1: Superoxide dismutase [Cu-Zn]



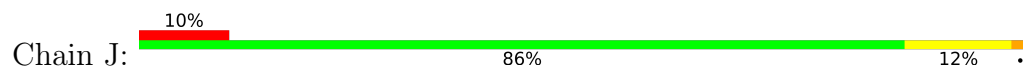
- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



- Molecule 1: Superoxide dismutase [Cu-Zn]



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	203.58Å 165.68Å 144.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.00-1.70) 97.6 (30.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 1.71Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.210 , 0.243 (Not available) , 0.244	Depositor DCC
R_{free} test set	13096 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12222	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% 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: CU1, SO4, 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	0.58	0/1140	1.41	5/1536 (0.3%)
1	B	0.60	0/1140	1.38	7/1536 (0.5%)
1	C	0.58	0/1140	1.61	14/1536 (0.9%)
1	D	0.57	0/1140	1.41	4/1536 (0.3%)
1	E	0.58	0/1140	1.43	7/1536 (0.5%)
1	F	0.58	0/1140	1.39	5/1536 (0.3%)
1	G	0.51	0/1140	1.46	9/1536 (0.6%)
1	H	0.53	0/1140	1.48	10/1536 (0.7%)
1	I	0.45	0/1140	1.35	4/1536 (0.3%)
1	J	0.49	0/1140	1.35	4/1536 (0.3%)
All	All	0.55	0/11400	1.43	69/15360 (0.4%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	VAL	CA-C-O	-8.80	114.73	121.68
1	H	25	SER	CA-C-O	8.33	129.81	120.90
1	G	45	PHE	CA-CB-CG	8.07	121.87	113.80
1	C	45	PHE	CA-CB-CG	7.93	121.73	113.80
1	C	87	VAL	O-C-N	7.41	129.01	122.12
1	C	124	ASP	CA-C-O	-7.05	112.66	120.69
1	I	45	PHE	CA-CB-CG	6.97	120.77	113.80
1	F	92	ASP	CA-CB-CG	-6.93	105.67	112.60
1	C	124	ASP	O-C-N	6.91	131.13	123.04
1	J	149	ILE	CA-C-N	-6.89	115.65	121.58
1	J	149	ILE	C-N-CA	-6.89	115.65	121.58
1	D	61	GLY	O-C-N	6.89	128.66	121.77
1	C	43	HIS	O-C-N	6.84	131.71	123.36
1	B	115	ARG	NE-CZ-NH2	6.76	125.28	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	108	GLY	CA-C-N	6.68	129.23	120.28
1	F	108	GLY	C-N-CA	6.68	129.23	120.28
1	B	108	GLY	CA-C-N	6.57	130.30	120.31
1	B	108	GLY	C-N-CA	6.57	130.30	120.31
1	B	24	GLU	CA-C-N	6.53	134.01	121.54
1	B	24	GLU	C-N-CA	6.53	134.01	121.54
1	C	125	ASP	CA-CB-CG	6.52	119.12	112.60
1	H	65	ASN	O-C-N	6.50	126.66	121.20
1	E	110	HIS	O-C-N	6.41	130.57	122.37
1	H	79	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	B	45	PHE	CA-CB-CG	6.25	120.05	113.80
1	F	109	ASP	O-C-N	6.14	128.63	122.12
1	G	46	HIS	CA-CB-CG	6.11	119.91	113.80
1	E	49	GLU	N-CA-C	6.03	117.85	111.28
1	E	108	GLY	CA-C-N	5.97	130.79	120.58
1	E	108	GLY	C-N-CA	5.97	130.79	120.58
1	A	38	LEU	CA-C-O	-5.97	114.20	121.36
1	E	115	ARG	NE-CZ-NH2	5.88	124.50	119.20
1	J	45	PHE	CA-CB-CG	5.88	119.67	113.80
1	C	110	HIS	CA-CB-CG	-5.85	107.95	113.80
1	H	65	ASN	CA-C-O	-5.78	115.40	121.29
1	E	113	ILE	O-C-N	-5.69	116.41	122.61
1	A	87	VAL	CA-C-O	-5.66	115.59	121.93
1	C	102	SER	CA-C-O	5.65	126.15	119.48
1	I	76	ASP	CA-C-N	5.61	128.12	120.54
1	I	76	ASP	C-N-CA	5.61	128.12	120.54
1	A	145	ALA	O-C-N	5.58	129.39	123.42
1	G	95	ALA	CA-C-N	-5.58	115.35	122.77
1	G	95	ALA	C-N-CA	-5.58	115.35	122.77
1	F	45	PHE	CA-CB-CG	5.50	119.30	113.80
1	G	24	GLU	CA-C-N	5.38	131.81	121.54
1	G	24	GLU	C-N-CA	5.38	131.81	121.54
1	D	45	PHE	CA-CB-CG	5.36	119.16	113.80
1	C	119	VAL	O-C-N	-5.36	117.67	123.14
1	C	105	SER	CA-C-O	-5.36	115.35	121.40
1	D	115	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	E	115	ARG	CD-NE-CZ	5.33	131.86	124.40
1	I	49	GLU	N-CA-C	5.30	116.75	111.07
1	A	117	LEU	CA-C-O	-5.27	114.58	120.54
1	A	45	PHE	CA-CB-CG	5.26	119.06	113.80
1	C	86	ASN	CA-C-N	-5.26	116.64	122.27
1	C	86	ASN	C-N-CA	-5.26	116.64	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	143	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	G	96	ASP	CA-CB-CG	-5.23	107.37	112.60
1	H	48	HIS	CA-C-N	5.19	127.19	120.44
1	H	48	HIS	C-N-CA	5.19	127.19	120.44
1	J	27	GLY	N-CA-C	5.17	118.49	112.23
1	C	92	ASP	CA-CB-CG	-5.15	107.45	112.60
1	G	120	HIS	CA-C-N	5.11	127.39	120.44
1	G	120	HIS	C-N-CA	5.11	127.39	120.44
1	D	110	HIS	CA-CB-CG	-5.08	108.72	113.80
1	H	113	ILE	O-C-N	-5.08	117.24	122.63
1	B	49	GLU	CA-C-O	-5.01	115.24	120.55
1	H	24	GLU	CA-C-N	5.01	127.30	120.54
1	H	24	GLU	C-N-CA	5.01	127.30	120.54

There are no chirality outliers.

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	1114	0	1079	6	0
1	B	1114	0	1079	8	0
1	C	1114	0	1079	29	0
1	D	1114	0	1079	14	0
1	E	1114	0	1079	10	0
1	F	1114	0	1079	10	0
1	G	1114	0	1079	25	0
1	H	1114	0	1079	10	0
1	I	1114	0	1079	22	0
1	J	1114	0	1079	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	B	5	0	0	0	0
4	J	10	0	0	1	0
5	A	131	0	0	2	0
5	B	141	0	0	2	0
5	C	57	0	0	1	0
5	D	133	0	0	4	0
5	E	133	0	0	4	0
5	F	126	0	0	0	0
5	G	55	0	0	2	0
5	H	107	0	0	0	0
5	I	60	0	0	2	0
5	J	104	0	0	1	0
All	All	12222	0	10790	140	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 7.

All (140) 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:57[B]:CYS:HG	1:B:146[B]:CYS:HG	0.88	0.85
1:G:57[B]:CYS:HG	1:G:146[B]:CYS:HG	0.85	0.83
1:H:57[B]:CYS:HG	1:H:146[B]:CYS:HG	0.95	0.81
1:J:57[B]:CYS:HG	1:J:146[B]:CYS:HG	0.86	0.81
1:J:24:GLU:OE1	1:J:28:PRO:HD2	1.84	0.78
1:A:57[B]:CYS:HG	1:A:146[B]:CYS:HG	0.89	0.75
1:D:75:LYS:HE3	5:D:519:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLU:HB2	1:C:144:LEU:HD21	1.70	0.72
1:E:23:LYS:HZ1	1:E:30:LYS:HD3	1.54	0.72
1:C:70:LYS:HE3	1:C:135:THR:HG21	1.70	0.71
1:I:131:ASN:ND2	1:I:134:SER:H	1.89	0.71
1:A:136:LYS:HD3	1:A:137:THR:HG23	1.74	0.69
1:C:40:GLU:OE2	1:C:91:LYS:HA	1.93	0.68
1:H:108:GLY:O	1:H:111:CYS:HB3	1.94	0.67
1:I:131:ASN:HD21	1:I:139:ASN:HD21	1.44	0.66
5:B:563:HOH:O	1:F:75:LYS:HE3	1.94	0.66
1:I:81:VAL:HG23	5:I:1359:HOH:O	1.96	0.65
1:D:2:THR:HG22	5:D:1488:HOH:O	1.97	0.64
1:F:23:LYS:HE3	1:F:30:LYS:HE3	1.79	0.64
1:C:67:LEU:HD22	1:C:69:ARG:NH1	2.11	0.63
1:G:3:LYS:HG2	1:G:21:GLU:HG2	1.80	0.62
1:C:40:GLU:HB2	1:C:90:ASP:O	2.01	0.61
1:J:21:GLU:OE1	1:J:23:LYS:HE3	2.01	0.61
1:J:24:GLU:OE1	1:J:27:GLY:HA3	2.02	0.60
1:C:57[B]:CYS:HG	1:C:146[B]:CYS:CB	2.15	0.59
1:H:30:LYS:HD3	1:H:100:GLU:HG3	1.83	0.59
1:C:23:LYS:HE2	1:C:24:GLU:HG2	1.85	0.59
1:G:153:GLN:HB2	1:H:50:PHE:CZ	2.38	0.58
1:G:76:ASP:OD1	1:G:128:LYS:HE2	2.04	0.57
1:A:57[B]:CYS:HG	1:A:146[B]:CYS:CB	2.18	0.57
1:H:57[B]:CYS:HG	1:H:146[B]:CYS:CB	2.18	0.57
1:E:100:GLU:HG2	5:E:814:HOH:O	2.05	0.56
1:I:24:GLU:HB2	1:I:27:GLY:HA3	1.87	0.56
1:D:23:LYS:HD3	1:D:23:LYS:N	2.20	0.56
1:D:36:LYS:HE3	5:D:1367:HOH:O	2.06	0.56
1:B:1:ALA:HB3	1:B:22:GLN:O	2.05	0.56
1:E:57[B]:CYS:HG	1:E:146[B]:CYS:CB	2.18	0.56
1:E:21:GLU:OE2	1:E:23:LYS:HE2	2.07	0.55
1:D:21:GLU:CD	1:D:23:LYS:HZ2	2.14	0.55
1:D:23:LYS:HE2	5:D:1281:HOH:O	2.05	0.55
1:I:131:ASN:O	1:I:135:THR:HG23	2.07	0.55
1:I:57[B]:CYS:HG	1:I:146[B]:CYS:HG	0.87	0.54
1:G:40:GLU:HG3	1:G:90:ASP:C	2.33	0.54
1:A:9:LYS:HG2	5:A:1378:HOH:O	2.07	0.53
1:E:23:LYS:HD2	5:E:698:HOH:O	2.09	0.52
1:C:49:GLU:O	1:C:115:ARG:HD3	2.10	0.52
1:G:133:GLU:HA	1:G:133:GLU:OE1	2.09	0.52
1:C:70:LYS:HD2	1:C:135:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57[B]:CYS:HG	1:G:146[B]:CYS:CB	2.22	0.52
1:G:69:ARG:CZ	1:G:78:GLU:HB2	2.40	0.51
1:C:69:ARG:HB3	1:C:78:GLU:OE1	2.10	0.51
1:C:21:GLU:HB2	1:C:32:TRP:CZ3	2.45	0.51
1:C:132:GLU:HG3	1:C:133:GLU:N	2.24	0.51
1:D:57[B]:CYS:HG	1:D:146[B]:CYS:CB	2.22	0.51
1:G:1:ALA:HA	1:G:22:GLN:O	2.10	0.51
1:C:81:VAL:HG23	5:C:1347:HOH:O	2.11	0.50
1:J:22:GLN:HB2	1:J:29:VAL:HG22	1.93	0.50
1:E:23:LYS:HE3	5:E:698:HOH:O	2.11	0.50
1:C:70:LYS:HB3	1:C:135:THR:HG22	1.92	0.50
1:C:74:PRO:HD3	1:C:85:GLY:CA	2.42	0.50
1:I:131:ASN:ND2	1:I:134:SER:HB2	2.27	0.50
1:I:80:HIS:HE1	1:I:136:LYS:O	1.94	0.50
1:J:21:GLU:CD	1:J:23:LYS:HZ1	2.20	0.50
1:I:57[B]:CYS:HG	1:I:146[B]:CYS:CB	2.21	0.49
1:I:126:LEU:O	1:I:128:LYS:HD2	2.12	0.49
1:G:69:ARG:NH1	1:G:78:GLU:HB2	2.27	0.49
1:C:131:ASN:OD1	1:C:134:SER:HB2	2.13	0.49
1:E:3:LYS:HE2	1:E:21:GLU:OE1	2.13	0.49
1:A:132:GLU:OE2	1:I:131:ASN:HB3	2.13	0.48
1:J:57[B]:CYS:HG	1:J:146[B]:CYS:CB	2.24	0.48
1:G:66:PRO:C	1:G:67:LEU:HD23	2.39	0.48
1:H:105:SER:O	1:H:111:CYS:HA	2.14	0.48
1:D:98:SER:HB2	1:F:132:GLU:HG2	1.94	0.47
1:C:80:HIS:HB2	1:C:83:ASP:CG	2.39	0.47
1:C:133:GLU:OE1	1:C:137:THR:OG1	2.30	0.47
1:I:70:LYS:HE3	1:I:70:LYS:HA	1.96	0.47
1:I:55:ALA:HB3	1:I:59:SER:OG	2.14	0.47
1:F:24:GLU:HA	1:F:24:GLU:OE2	2.14	0.47
1:J:136:LYS:HE3	5:J:1040:HOH:O	2.13	0.47
1:G:21:GLU:HB2	1:G:32:TRP:CZ3	2.50	0.46
1:C:21:GLU:HB2	1:C:32:TRP:HZ3	1.79	0.46
1:G:132:GLU:HG2	1:G:132:GLU:O	2.15	0.46
1:I:131:ASN:HD22	1:I:134:SER:H	1.62	0.46
1:C:132:GLU:C	1:C:135:THR:HG1	2.21	0.46
1:C:129:GLY:HA3	1:C:134:SER:HB2	1.96	0.46
1:G:110:HIS:HB2	5:G:1404:HOH:O	2.16	0.46
1:C:50:PHE:CZ	1:D:153:GLN:HB2	2.50	0.46
1:G:99:ILE:HD11	5:G:1235:HOH:O	2.16	0.46
1:G:69:ARG:NH2	1:G:78:GLU:OE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:HIS:HB2	1:B:83:ASP:CG	2.42	0.45
1:I:8:LEU:O	1:I:9:LYS:HG3	2.16	0.45
1:B:57[B]:CYS:CB	1:B:146[B]:CYS:HG	2.27	0.45
1:G:70:LYS:HD2	1:G:135:THR:HB	1.98	0.45
1:I:69:ARG:HG3	1:I:69:ARG:HH21	1.82	0.45
1:G:3:LYS:HG2	1:G:21:GLU:CG	2.47	0.45
1:B:24:GLU:OE1	1:B:27:GLY:N	2.50	0.45
1:B:25:SER:OG	1:B:26:ASN:ND2	2.50	0.45
1:J:109:ASP:N	1:J:109:ASP:OD1	2.50	0.45
1:C:76:ASP:OD2	1:C:76:ASP:N	2.50	0.45
1:C:122:LYS:NZ	1:C:139:ASN:O	2.50	0.45
1:E:109:ASP:N	5:E:806:HOH:O	2.50	0.44
1:G:71:HIS:HB2	1:G:80:HIS:CE1	2.52	0.44
1:G:132:GLU:HG2	1:G:136:LYS:NZ	2.32	0.44
1:G:134:SER:HB2	1:G:139:ASN:ND2	2.33	0.44
1:C:121:GLU:HA	1:C:144:LEU:HD11	1.99	0.44
1:J:71:HIS:HB2	1:J:80:HIS:CE1	2.52	0.44
1:C:75:LYS:HB2	1:H:153:GLN:OE1	2.17	0.44
1:J:67:LEU:N	1:J:67:LEU:HD23	2.33	0.44
1:D:38:LEU:O	1:D:93:GLY:HA2	2.17	0.44
1:D:75:LYS:HZ3	1:F:128:LYS:HD2	1.83	0.43
1:G:134:SER:HB2	1:G:139:ASN:HD21	1.83	0.43
1:E:69:ARG:HD3	1:E:78:GLU:OE2	2.18	0.43
1:I:52:ASP:O	1:I:59:SER:HB2	2.18	0.43
1:H:71:HIS:HB2	1:H:80:HIS:CE1	2.54	0.43
1:I:76:ASP:O	1:I:79:ARG:HG2	2.19	0.43
1:D:75:LYS:HE2	1:F:128:LYS:HG2	1.99	0.43
1:E:21:GLU:OE2	1:E:30:LYS:NZ	2.52	0.43
1:H:26:ASN:OD1	1:H:26:ASN:N	2.50	0.43
1:I:77:GLU:CD	1:I:78:GLU:H	2.27	0.42
1:F:57[B]:CYS:HG	1:F:146[B]:CYS:CB	2.28	0.42
1:J:39:THR:HG22	4:J:302:SO4:O1	2.19	0.42
1:C:76:ASP:OD1	1:C:128:LYS:NZ	2.50	0.42
1:G:34:SER:HB3	1:G:96:ASP:OD1	2.20	0.42
1:A:110:HIS:HD2	5:A:1311:HOH:O	2.03	0.42
1:B:23:LYS:HG2	5:B:719:HOH:O	2.19	0.42
1:G:98:SER:C	1:G:99:ILE:HD13	2.45	0.42
1:I:133:GLU:HA	1:I:136:LYS:HE3	2.01	0.41
1:D:80:HIS:HB2	1:D:83:ASP:CG	2.45	0.41
1:J:106:LEU:HD22	1:J:113:ILE:HD11	2.03	0.41
1:C:74:PRO:HD3	1:C:85:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:GLY:N	1:C:134:SER:OG	2.51	0.41
1:F:99:ILE:HD13	1:F:99:ILE:HG21	1.89	0.41
1:B:24:GLU:OE1	1:B:26:ASN:N	2.49	0.41
1:H:22:GLN:HG2	1:H:24:GLU:O	2.21	0.41
1:G:2:THR:HG22	1:G:3:LYS:N	2.36	0.41
1:I:27:GLY:HA3	5:I:1418:HOH:O	2.20	0.40
1:F:71:HIS:HB2	1:F:80:HIS:CE1	2.56	0.40
1:I:71:HIS:HB2	1:I:80:HIS:CE1	2.56	0.40
1:D:48:HIS:O	1:D:115:ARG:HB3	2.22	0.40
1:F:23:LYS:CE	1:F:30:LYS:HE3	2.49	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	153/153 (100%)	153 (100%)	0	0	100	100
1	B	153/153 (100%)	152 (99%)	0	1 (1%)	18	7
1	C	153/153 (100%)	147 (96%)	6 (4%)	0	100	100
1	D	153/153 (100%)	152 (99%)	1 (1%)	0	100	100
1	E	153/153 (100%)	151 (99%)	2 (1%)	0	100	100
1	F	153/153 (100%)	153 (100%)	0	0	100	100
1	G	153/153 (100%)	147 (96%)	4 (3%)	2 (1%)	9	2
1	H	67/153 (44%)	67 (100%)	0	0	100	100
1	J	57/153 (37%)	55 (96%)	2 (4%)	0	100	100
All	All	1195/1377 (87%)	1177 (98%)	15 (1%)	3 (0%)	36	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	SER
1	G	25	SER
1	G	132	GLU

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	J	120/118 (102%)	115 (96%)	5 (4%)	26 11

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	2	THR
1	J	24	GLU
1	J	36	LYS
1	J	59	SER
1	J	109	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 23 ligands modelled in this entry, 20 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	J	301	-	4,4,4	0.39	0	6,6,6	0.15	0
4	SO4	J	302	-	4,4,4	0.38	0	6,6,6	0.10	0
4	SO4	B	300	-	4,4,4	0.43	0	6,6,6	0.36	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	302	SO4	1	0

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	153/153 (100%)	0.41	9 (5%)	28 31	17, 28, 46, 59	2 (1%)
1	B	153/153 (100%)	0.11	9 (5%)	28 31	17, 24, 49, 71	2 (1%)
1	C	153/153 (100%)	2.16	81 (52%)	0 0	22, 39, 70, 89	2 (1%)
1	D	153/153 (100%)	0.22	9 (5%)	28 31	17, 24, 48, 64	2 (1%)
1	E	153/153 (100%)	0.26	8 (5%)	33 36	16, 25, 44, 64	2 (1%)
1	F	153/153 (100%)	0.27	12 (7%)	19 20	17, 25, 50, 76	2 (1%)
1	G	153/153 (100%)	1.72	52 (33%)	1 1	24, 39, 75, 81	2 (1%)
1	H	153/153 (100%)	0.48	12 (7%)	19 20	21, 29, 54, 86	2 (1%)
1	I	153/153 (100%)	1.18	34 (22%)	2 2	22, 37, 71, 95	2 (1%)
1	J	153/153 (100%)	0.60	15 (9%)	13 13	21, 30, 56, 88	2 (1%)
All	All	1530/1530 (100%)	0.74	241 (15%)	5 4	16, 30, 60, 95	20 (1%)

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1	ALA	7.4
1	C	69	ARG	6.9
1	C	129	GLY	6.7
1	F	1	ALA	6.1
1	C	1	ALA	6.0
1	D	1	ALA	6.0
1	C	135	THR	5.7
1	C	128	LYS	5.6
1	C	109	ASP	5.5
1	D	26	ASN	5.5
1	B	1	ALA	5.5
1	C	75	LYS	5.5
1	I	1	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
1	G	107	SER	5.3
1	C	77	GLU	5.3
1	H	1	ALA	5.3
1	G	136	LYS	5.2
1	C	123	ALA	5.2
1	G	133	GLU	5.0
1	J	24	GLU	4.9
1	G	25	SER	4.9
1	G	108	GLY	4.8
1	C	78	GLU	4.8
1	F	26	ASN	4.8
1	C	76	ASP	4.7
1	G	76	ASP	4.6
1	B	23	LYS	4.6
1	G	26	ASN	4.6
1	C	72	GLY	4.5
1	C	42	LEU	4.4
1	I	25	SER	4.4
1	I	108	GLY	4.4
1	B	25	SER	4.4
1	H	109	ASP	4.4
1	C	39	THR	4.4
1	G	70	LYS	4.4
1	C	98	SER	4.3
1	G	1	ALA	4.3
1	I	107	SER	4.3
1	C	67	LEU	4.3
1	G	99	ILE	4.2
1	J	25	SER	4.2
1	J	23	LYS	4.2
1	G	130	GLY	4.1
1	I	131	ASN	4.1
1	E	109	ASP	4.1
1	G	67	LEU	4.0
1	H	111	CYS	4.0
1	B	24	GLU	4.0
1	I	128	LYS	3.9
1	C	130	GLY	3.9
1	E	1	ALA	3.9
1	E	108	GLY	3.9
1	C	122	LYS	3.9
1	I	130	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	23	LYS	3.8
1	H	110	HIS	3.8
1	C	99	ILE	3.8
1	C	94	VAL	3.8
1	G	109	ASP	3.7
1	I	24	GLU	3.7
1	I	77	GLU	3.7
1	H	2	THR	3.7
1	I	2	THR	3.7
1	A	130	GLY	3.7
1	I	75	LYS	3.6
1	D	23	LYS	3.5
1	B	26	ASN	3.5
1	C	95	ALA	3.5
1	J	2	THR	3.5
1	C	85	GLY	3.5
1	A	109	ASP	3.4
1	I	136	LYS	3.4
1	J	107	SER	3.4
1	C	126	LEU	3.4
1	D	2	THR	3.4
1	J	11	ASP	3.4
1	I	110	HIS	3.4
1	G	98	SER	3.3
1	F	77	GLU	3.3
1	A	1	ALA	3.3
1	G	12	GLY	3.3
1	C	138	GLY	3.2
1	B	2	THR	3.2
1	C	2	THR	3.2
1	C	68	SER	3.2
1	C	133	GLU	3.2
1	D	25	SER	3.2
1	G	69	ARG	3.2
1	I	132	GLU	3.2
1	I	129	GLY	3.2
1	G	78	GLU	3.2
1	B	70	LYS	3.2
1	C	23	LYS	3.2
1	G	68	SER	3.2
1	C	137	THR	3.2
1	F	2	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	77	GLU	3.2
1	C	124	ASP	3.1
1	C	131	ASN	3.1
1	A	110	HIS	3.1
1	G	72	GLY	3.1
1	G	139	ASN	3.1
1	I	26	ASN	3.1
1	G	2	THR	3.1
1	H	108	GLY	3.0
1	G	131	ASN	3.0
1	C	84	LEU	3.0
1	J	26	ASN	3.0
1	G	129	GLY	3.0
1	C	125	ASP	2.9
1	H	32	TRP	2.9
1	F	23	LYS	2.9
1	C	31	VAL	2.9
1	C	136	LYS	2.9
1	C	110	HIS	2.9
1	I	67	LEU	2.9
1	C	30	LYS	2.9
1	C	71	HIS	2.9
1	G	132	GLU	2.8
1	E	23	LYS	2.8
1	C	36	LYS	2.8
1	J	75	LYS	2.8
1	I	111	CYS	2.8
1	C	88	THR	2.8
1	I	137	THR	2.8
1	B	11	ASP	2.8
1	C	96	ASP	2.8
1	B	27	GLY	2.8
1	H	26	ASN	2.8
1	I	72	GLY	2.8
1	G	103	VAL	2.7
1	J	109	ASP	2.7
1	C	90	ASP	2.7
1	J	110	HIS	2.7
1	C	40	GLU	2.7
1	C	103	VAL	2.7
1	I	58	THR	2.7
1	I	103	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	74	PRO	2.6
1	C	83	ASP	2.6
1	I	66	PRO	2.6
1	C	44	GLY	2.6
1	C	127	GLY	2.6
1	F	69	ARG	2.6
1	G	138	GLY	2.6
1	H	132	GLU	2.6
1	D	153	GLN	2.6
1	C	70	LYS	2.6
1	C	104	ILE	2.6
1	H	25	SER	2.6
1	C	153	GLN	2.5
1	F	67	LEU	2.5
1	G	134	SER	2.5
1	C	81	VAL	2.5
1	C	100	GLU	2.5
1	C	62	PRO	2.5
1	C	93	GLY	2.5
1	I	127	GLY	2.5
1	C	91	LYS	2.5
1	G	122	LYS	2.5
1	C	86	ASN	2.5
1	C	132	GLU	2.5
1	E	132	GLU	2.5
1	I	55	ALA	2.5
1	E	110	HIS	2.5
1	E	70	LYS	2.5
1	C	34	SER	2.5
1	I	153	GLN	2.5
1	C	144	LEU	2.5
1	D	67	LEU	2.5
1	H	23	LYS	2.5
1	I	27	GLY	2.5
1	D	69	ARG	2.5
1	F	24	GLU	2.5
1	G	96	ASP	2.4
1	C	21	GLU	2.4
1	G	71	HIS	2.4
1	I	133	GLU	2.4
1	C	89	ALA	2.4
1	I	135	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	26	ASN	2.4
1	F	109	ASP	2.4
1	C	27	GLY	2.4
1	C	82	GLY	2.4
1	C	134	SER	2.4
1	G	102	SER	2.4
1	G	125	ASP	2.4
1	G	27	GLY	2.4
1	J	108	GLY	2.4
1	C	139	ASN	2.4
1	G	64	PHE	2.4
1	C	28	PRO	2.3
1	C	140	ALA	2.3
1	G	137	THR	2.3
1	G	127	GLY	2.3
1	G	101	ASP	2.3
1	G	94	VAL	2.3
1	C	33	GLY	2.3
1	A	11	ASP	2.3
1	G	11	ASP	2.3
1	G	28	PRO	2.3
1	C	46	HIS	2.3
1	I	70	LYS	2.3
1	J	113	ILE	2.3
1	A	2	THR	2.2
1	A	131	ASN	2.2
1	C	38	LEU	2.2
1	E	67	LEU	2.2
1	C	29	VAL	2.2
1	I	11	ASP	2.2
1	A	129	GLY	2.2
1	G	110	HIS	2.2
1	J	151	ILE	2.2
1	C	97	VAL	2.2
1	C	92	ASP	2.2
1	H	153	GLN	2.2
1	C	79	ARG	2.2
1	G	128	LYS	2.2
1	C	17	ILE	2.2
1	C	119	VAL	2.1
1	G	100	GLU	2.1
1	A	135	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	87	VAL	2.1
1	G	29	VAL	2.1
1	C	63	HIS	2.1
1	I	138	GLY	2.1
1	F	91	LYS	2.1
1	D	75	LYS	2.1
1	G	30	LYS	2.1
1	G	153	GLN	2.1
1	C	32	TRP	2.1
1	I	9	LYS	2.1
1	F	92	ASP	2.0
1	I	109	ASP	2.0
1	G	57[A]	CYS	2.0
1	G	126	LEU	2.0
1	G	24	GLU	2.0
1	G	22	GLN	2.0
1	J	153	GLN	2.0
1	F	9	LYS	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
4	SO4	J	302	5/5	0.69	0.17	52,105,121,128	0
4	SO4	J	301	5/5	0.79	0.17	56,83,87,88	0
4	SO4	B	300	5/5	0.79	0.15	43,55,64,85	0
3	ZN	I	201	1/1	0.99	0.03	40,40,40,40	0
2	CU1	G	200	1/1	0.99	0.05	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	C	201	1/1	0.99	0.03	46,46,46,46	0
3	ZN	G	201	1/1	0.99	0.03	44,44,44,44	0
2	CU1	H	200	1/1	1.00	0.02	25,25,25,25	0
2	CU1	I	200	1/1	1.00	0.04	35,35,35,35	0
2	CU1	J	200	1/1	1.00	0.02	24,24,24,24	0
3	ZN	A	201	1/1	1.00	0.01	25,25,25,25	0
3	ZN	B	201	1/1	1.00	0.01	20,20,20,20	0
2	CU1	B	200	1/1	1.00	0.03	21,21,21,21	0
3	ZN	D	201	1/1	1.00	0.01	20,20,20,20	0
3	ZN	E	201	1/1	1.00	0.01	22,22,22,22	0
3	ZN	F	201	1/1	1.00	0.01	21,21,21,21	0
2	CU1	C	200	1/1	1.00	0.03	40,40,40,40	0
3	ZN	H	201	1/1	1.00	0.01	24,24,24,24	0
2	CU1	D	200	1/1	1.00	0.03	22,22,22,22	0
3	ZN	J	201	1/1	1.00	0.02	23,23,23,23	0
2	CU1	E	200	1/1	1.00	0.03	22,22,22,22	0
2	CU1	F	200	1/1	1.00	0.03	21,21,21,21	0
2	CU1	A	200	1/1	1.00	0.03	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.