



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:07 AM UTC

PDB ID : 4FXO / pdb_00004fxo
Title : Zinc-mediated allosteric inhibition of caspase-6
Authors : Velazquez-Delgado, E.M.; Hardy, J.A.
Deposited on : 2012-07-03
Resolution : 2.85 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

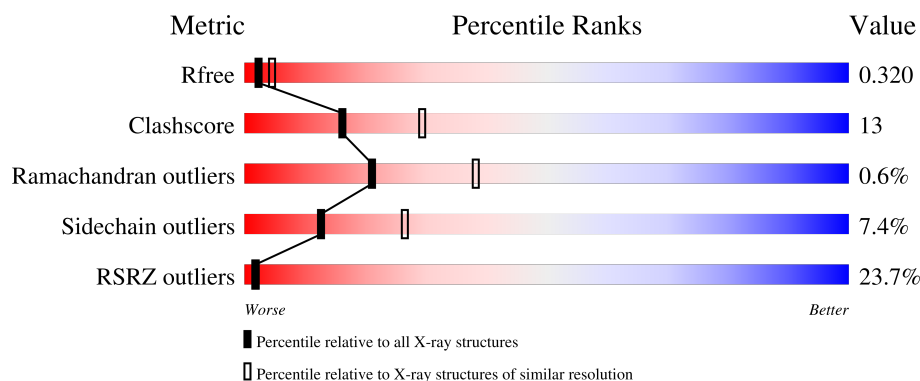
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	299	15% 54% 17% • 27%
1	B	299	19% 57% 16% • 24%
1	C	299	18% 49% 23% • 26%
1	D	299	18% 49% 22% • 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6781 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 Caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	1	0
			1692	1086	286	306	14			
1	B	227	Total	C	N	O	S	0	0	0
			1731	1106	300	311	14			
1	C	220	Total	C	N	O	S	0	0	0
			1680	1074	289	304	13			
1	D	220	Total	C	N	O	S	0	0	0
			1666	1064	286	303	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	HIS	-	expression tag	UNP P55212
A	295	HIS	-	expression tag	UNP P55212
A	296	HIS	-	expression tag	UNP P55212
A	297	HIS	-	expression tag	UNP P55212
A	298	HIS	-	expression tag	UNP P55212
A	299	HIS	-	expression tag	UNP P55212
B	294	HIS	-	expression tag	UNP P55212
B	295	HIS	-	expression tag	UNP P55212
B	296	HIS	-	expression tag	UNP P55212
B	297	HIS	-	expression tag	UNP P55212
B	298	HIS	-	expression tag	UNP P55212
B	299	HIS	-	expression tag	UNP P55212
C	294	HIS	-	expression tag	UNP P55212
C	295	HIS	-	expression tag	UNP P55212
C	296	HIS	-	expression tag	UNP P55212
C	297	HIS	-	expression tag	UNP P55212
C	298	HIS	-	expression tag	UNP P55212
C	299	HIS	-	expression tag	UNP P55212
D	294	HIS	-	expression tag	UNP P55212
D	295	HIS	-	expression tag	UNP P55212
D	296	HIS	-	expression tag	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	297	HIS	-	expression tag	UNP P55212
D	298	HIS	-	expression tag	UNP P55212
D	299	HIS	-	expression tag	UNP P55212

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

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

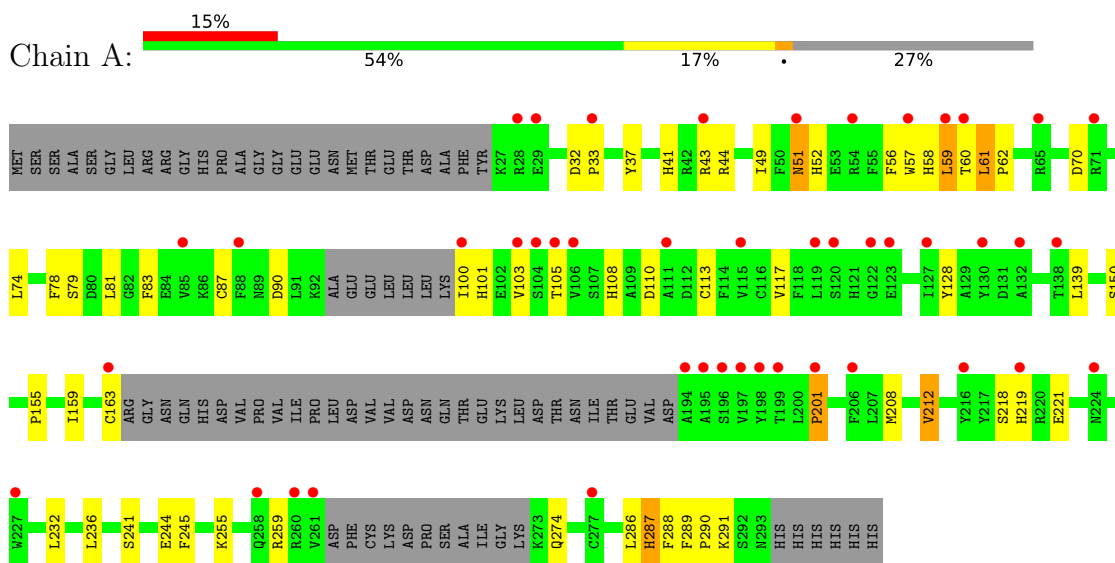
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		

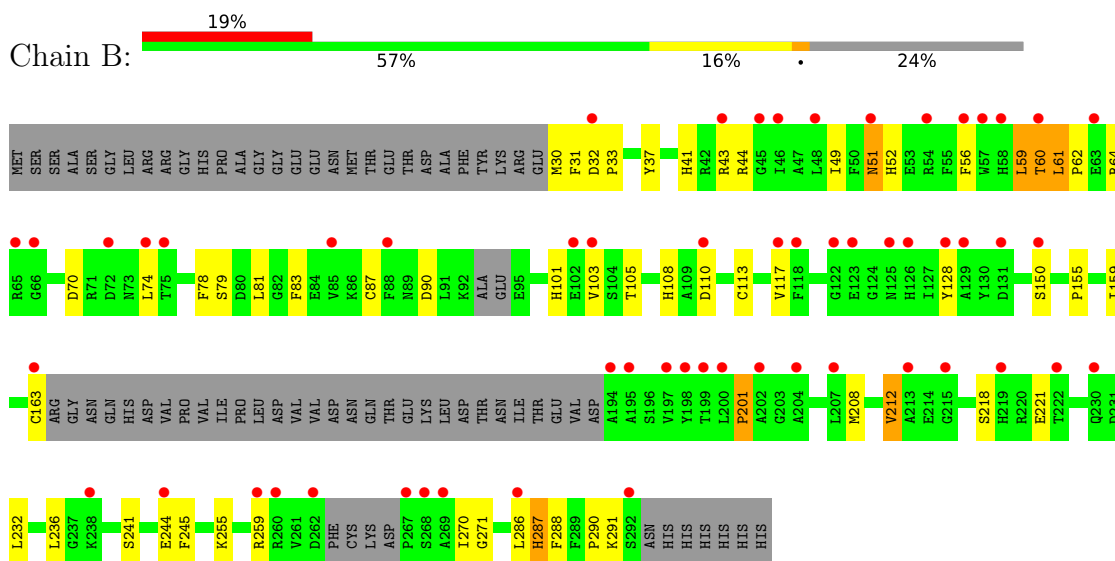
3 Residue-property plots [i](#)

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.

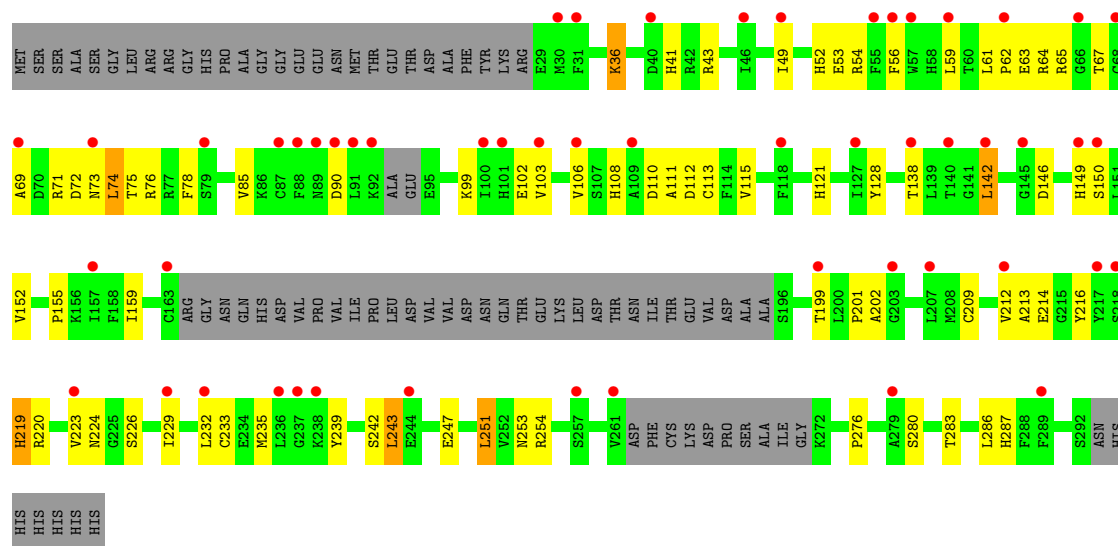
• Molecule 1: Caspase-6



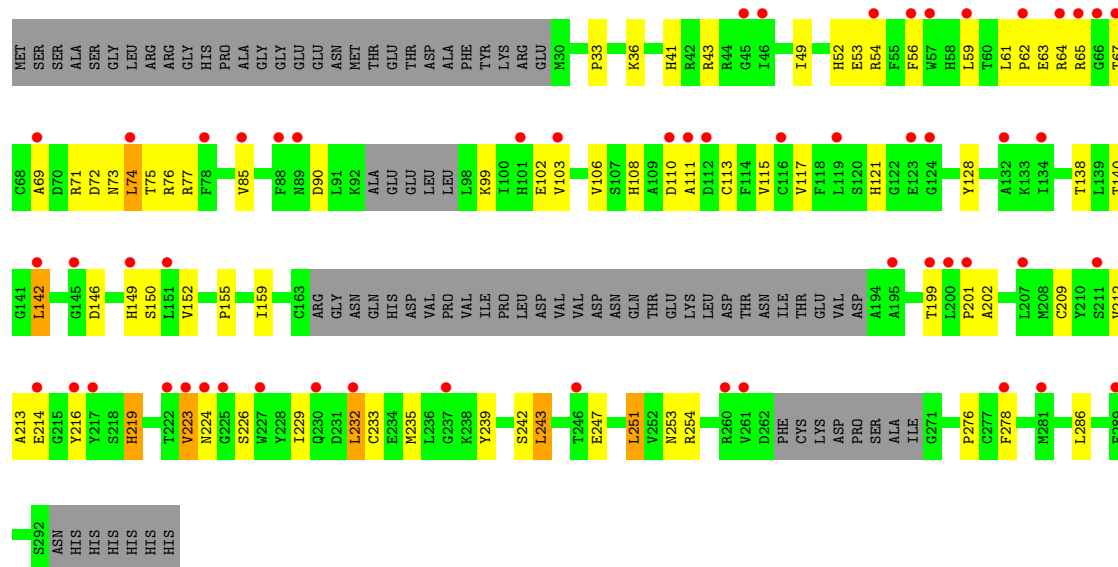
• Molecule 1: Caspase-6



• Molecule 1: Caspase-6



● Molecule 1: Caspase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.70Å 90.86Å 85.76Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	84.2 (30.00-2.85) 99.2 (30.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.233 0.302 , 0.320	Depositor DCC
R_{free} test set	4395 reflections (16.47%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.080 for h,-k,-l	Xtriage
Reported twinning fraction	0.401 for H, K, L 0.363 for -h,-k,l 0.119 for -H, -L, -K 0.117 for -H, L, K	Depositor
Outliers	0 of 23471 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6781	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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	0.37	0/1734	0.71	0/2343
1	B	0.37	0/1770	0.71	0/2389
1	C	0.41	0/1717	0.72	0/2317
1	D	0.41	0/1704	0.72	0/2304
All	All	0.39	0/6925	0.71	0/9353

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	VAL	Peptide
1	C	65	ARG	Peptide
1	D	223	VAL	Peptide
1	D	65	ARG	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	1692	0	1584	37	0
1	B	1731	0	1619	34	0
1	C	1680	0	1561	54	0
1	D	1666	0	1529	55	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
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	6781	0	6293	171	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 13.

All (171) 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:D:74:LEU:HD12	1:D:233:CYS:SG	1.93	1.08
1:C:67:THR:OG1	1:C:121:HIS:HE1	1.39	1.06
1:D:71:ARG:O	1:D:75:THR:HG22	1.57	1.05
1:C:71:ARG:O	1:C:75:THR:HG22	1.57	1.04
1:D:67:THR:OG1	1:D:121:HIS:HE1	1.42	0.99
1:D:213:ALA:O	1:D:216:TYR:HB3	1.63	0.97
1:C:67:THR:OG1	1:C:121:HIS:CE1	2.20	0.94
1:C:74:LEU:HD12	1:C:229:ILE:HG23	1.53	0.91
1:D:67:THR:OG1	1:D:121:HIS:CE1	2.22	0.91
1:D:74:LEU:HD13	1:D:229:ILE:HG23	1.64	0.79
1:B:270:ILE:H	1:B:271:GLY:HA2	1.49	0.77
1:C:74:LEU:CD1	1:C:229:ILE:HG23	2.19	0.72
1:C:74:LEU:CD2	1:C:78:PHE:HE2	2.02	0.72
1:C:74:LEU:HD12	1:C:229:ILE:CG2	2.19	0.71
1:B:49:ILE:HB	1:B:87:CYS:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:THR:O	1:D:142:LEU:HB2	1.92	0.68
1:C:74:LEU:CD2	1:C:78:PHE:CE2	2.76	0.68
1:D:53:GLU:OE2	1:D:121:HIS:NE2	2.26	0.68
1:D:69:ALA:HB3	1:D:224:ASN:O	1.93	0.68
1:A:49:ILE:HB	1:A:87:CYS:HB3	1.75	0.67
1:C:53:GLU:OE2	1:C:121:HIS:NE2	2.28	0.67
1:C:138:THR:O	1:C:142:LEU:HB2	1.96	0.65
1:B:270:ILE:N	1:B:271:GLY:HA2	2.12	0.64
1:C:54:ARG:HD3	1:C:90:ASP:HB2	1.80	0.64
1:D:54:ARG:HD3	1:D:90:ASP:HB2	1.79	0.63
1:A:244:GLU:CD	1:A:287:HIS:HD1	2.06	0.63
1:C:41:HIS:ND1	1:C:112:ASP:OD1	2.31	0.63
1:A:289:PHE:HE1	1:D:242:SER:CB	2.12	0.63
1:B:244:GLU:CD	1:B:287:HIS:HD1	2.06	0.62
1:C:72:ASP:HA	1:C:75:THR:CG2	2.29	0.62
1:D:72:ASP:HA	1:D:75:THR:CG2	2.29	0.62
1:C:69:ALA:O	1:C:73:ASN:HB2	2.00	0.61
1:C:69:ALA:HB3	1:C:224:ASN:O	2.01	0.61
1:C:99:LYS:O	1:C:102:GLU:HG2	2.01	0.61
1:D:243:LEU:HD23	1:D:247:GLU:CD	2.26	0.60
1:D:69:ALA:O	1:D:73:ASN:HB2	2.00	0.60
1:C:213:ALA:O	1:C:216:TYR:CB	2.49	0.60
1:A:113:CYS:HB3	1:A:155:PRO:HG2	1.84	0.59
1:C:61:LEU:HA	1:C:64:ARG:HB3	1.83	0.59
1:B:113:CYS:HB3	1:B:155:PRO:HG2	1.85	0.59
1:C:74:LEU:HD23	1:C:78:PHE:CE2	2.37	0.59
1:D:52:HIS:HD2	1:D:90:ASP:OD2	1.86	0.59
1:C:243:LEU:HD23	1:C:247:GLU:CD	2.28	0.58
1:A:201:PRO:HG2	1:A:208:MET:HE2	1.86	0.58
1:B:51:ASN:H	1:B:51:ASN:HD22	1.52	0.57
1:C:52:HIS:HD2	1:C:90:ASP:OD2	1.87	0.57
1:A:51:ASN:H	1:A:51:ASN:HD22	1.52	0.57
1:B:201:PRO:HG2	1:B:208:MET:HE2	1.85	0.57
1:D:49:ILE:HG21	1:D:71:ARG:HG3	1.87	0.57
1:A:101:HIS:O	1:A:105:THR:N	2.38	0.56
1:D:64:ARG:HD3	1:D:64:ARG:C	2.30	0.56
1:C:242:SER:C	1:C:287:HIS:HE2	2.14	0.56
1:C:61:LEU:HD12	1:C:64:ARG:HG2	1.88	0.56
1:C:202:ALA:HB2	1:D:214:GLU:O	2.06	0.56
1:D:251:LEU:HD23	1:D:254:ARG:HH22	1.69	0.56
1:C:49:ILE:HG21	1:C:71:ARG:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:N	1:D:62:PRO:HD2	2.21	0.56
1:C:61:LEU:N	1:C:62:PRO:HD2	2.21	0.55
1:B:43:ARG:HH21	1:B:110:ASP:HB2	1.72	0.55
1:D:108:HIS:H	1:D:150:SER:HB2	1.72	0.55
1:C:108:HIS:H	1:C:150:SER:HB2	1.72	0.54
1:C:247:GLU:O	1:C:251:LEU:HD12	2.07	0.54
1:B:101:HIS:O	1:B:105:THR:N	2.38	0.54
1:A:43:ARG:HH21	1:A:110:ASP:HB2	1.72	0.54
1:B:52:HIS:HE1	1:B:128:TYR:O	1.91	0.54
1:A:289:PHE:HE1	1:D:242:SER:HB2	1.72	0.53
1:B:41:HIS:O	1:B:291:LYS:NZ	2.41	0.53
1:C:243:LEU:CD2	1:C:247:GLU:CD	2.81	0.53
1:D:212:VAL:CG2	1:D:216:TYR:HB2	2.38	0.53
1:A:41:HIS:O	1:A:291:LYS:NZ	2.41	0.53
1:C:251:LEU:HD23	1:C:254:ARG:HH22	1.74	0.53
1:B:74:LEU:HD13	1:B:117:VAL:HG11	1.91	0.53
1:D:212:VAL:HG22	1:D:216:TYR:HB2	1.90	0.53
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.90	0.53
1:B:52:HIS:HD2	1:B:90:ASP:OD2	1.93	0.53
1:C:74:LEU:HG	1:C:233:CYS:SG	2.48	0.53
1:D:72:ASP:HA	1:D:75:THR:HG22	1.91	0.53
1:A:52:HIS:HE1	1:A:128:TYR:O	1.91	0.52
1:C:72:ASP:HA	1:C:75:THR:HG22	1.91	0.52
1:D:247:GLU:O	1:D:251:LEU:HD12	2.09	0.52
1:A:100:ILE:HD11	1:A:139:LEU:HD13	1.92	0.52
1:A:259:ARG:O	1:A:259:ARG:HG2	2.10	0.52
1:A:108:HIS:H	1:A:150:SER:CB	2.24	0.51
1:C:214:GLU:O	1:D:202:ALA:HB2	2.09	0.51
1:A:245:PHE:HB2	1:A:286:LEU:HD23	1.93	0.51
1:A:52:HIS:HD2	1:A:90:ASP:OD2	1.93	0.51
1:B:60:THR:HB	1:B:62:PRO:HD2	1.92	0.51
1:A:60:THR:HB	1:A:62:PRO:HD2	1.93	0.51
1:B:259:ARG:O	1:B:259:ARG:HG2	2.10	0.51
1:A:51:ASN:H	1:A:51:ASN:ND2	2.09	0.50
1:A:159:ILE:HD13	1:A:232[A]:LEU:HD21	1.94	0.50
1:B:51:ASN:H	1:B:51:ASN:ND2	2.09	0.50
1:B:108:HIS:H	1:B:150:SER:CB	2.24	0.50
1:A:56:PHE:CD2	1:A:59:LEU:HD12	2.48	0.49
1:B:245:PHE:HB2	1:B:286:LEU:HD23	1.95	0.49
1:D:71:ARG:O	1:D:75:THR:CG2	2.46	0.49
1:C:239:TYR:HB3	1:C:243:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PRO:HG2	1:C:36:LYS:HE3	1.94	0.48
1:B:286:LEU:HD21	1:B:288:PHE:CZ	2.48	0.48
1:A:286:LEU:HD21	1:A:288:PHE:CZ	2.48	0.48
1:C:113:CYS:SG	1:C:155:PRO:HG2	2.54	0.48
1:C:239:TYR:HB3	1:C:243:LEU:CD1	2.44	0.47
1:B:59:LEU:CD2	1:B:64:ARG:HB2	2.45	0.47
1:D:213:ALA:O	1:D:216:TYR:CB	2.50	0.47
1:A:241:SER:HB2	1:A:290:PRO:HD3	1.97	0.47
1:D:74:LEU:HD22	1:D:117:VAL:HG11	1.95	0.47
1:D:77:ARG:HH11	1:D:233:CYS:HB3	1.79	0.47
1:D:113:CYS:SG	1:D:155:PRO:HG2	2.55	0.47
1:C:102:GLU:O	1:C:106:VAL:HG23	2.15	0.46
1:D:219:HIS:CE1	1:D:226:SER:HB2	2.51	0.46
1:B:241:SER:HB2	1:B:290:PRO:HD3	1.96	0.46
1:C:71:ARG:O	1:C:75:THR:CG2	2.46	0.46
1:C:43:ARG:O	1:C:111:ALA:HA	2.16	0.46
1:C:280:SER:HB3	1:D:278:PHE:CZ	2.51	0.45
1:C:283:THR:HB	1:D:254:ARG:HG3	1.98	0.45
1:C:219:HIS:CE1	1:C:226:SER:HB2	2.51	0.45
1:D:43:ARG:O	1:D:111:ALA:HA	2.17	0.45
1:A:51:ASN:HD22	1:A:51:ASN:N	2.14	0.44
1:D:159:ILE:HA	1:D:209:CYS:HB2	2.00	0.44
1:D:239:TYR:HB3	1:D:243:LEU:HD13	1.99	0.44
1:A:32:ASP:HA	1:A:33:PRO:HD2	1.86	0.44
1:A:78:PHE:O	1:A:83:PHE:HB2	2.18	0.44
1:B:51:ASN:HD22	1:B:51:ASN:N	2.14	0.44
1:C:251:LEU:HD21	1:D:33:PRO:HA	2.00	0.44
1:D:74:LEU:CD2	1:D:117:VAL:HG21	2.47	0.44
1:B:159:ILE:HD13	1:B:232:LEU:HD21	1.99	0.44
1:D:102:GLU:O	1:D:106:VAL:HG23	2.17	0.44
1:B:56:PHE:CD2	1:B:59:LEU:HD12	2.53	0.43
1:B:78:PHE:O	1:B:83:PHE:HB2	2.18	0.43
1:C:159:ILE:HA	1:C:209:CYS:HB2	1.99	0.43
1:D:56:PHE:CE1	1:D:121:HIS:HB2	2.54	0.43
1:D:232:LEU:HD12	1:D:232:LEU:C	2.44	0.43
1:C:74:LEU:HD23	1:C:78:PHE:CD2	2.54	0.43
1:B:44:ARG:HD2	1:B:81:LEU:O	2.19	0.42
1:B:212:VAL:HG21	1:B:218:SER:HB2	2.01	0.42
1:B:236:LEU:HD21	1:B:245:PHE:HE1	1.85	0.42
1:D:243:LEU:HD23	1:D:247:GLU:CG	2.49	0.42
1:C:56:PHE:CE1	1:C:121:HIS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:HA	1:A:58:HIS:HA	1.70	0.42
1:A:212:VAL:HG21	1:A:218:SER:HB2	2.01	0.42
1:B:70:ASP:OD2	1:B:221:GLU:OE2	2.38	0.42
1:A:44:ARG:HD2	1:A:81:LEU:O	2.19	0.42
1:A:289:PHE:CE1	1:D:242:SER:CB	2.97	0.42
1:A:70:ASP:OD2	1:A:221:GLU:OE2	2.38	0.42
1:D:253:ASN:HA	1:D:276:PRO:HG2	2.01	0.42
1:D:59:LEU:HD11	1:D:63:GLU:HB2	2.02	0.42
1:D:243:LEU:CD2	1:D:247:GLU:CD	2.91	0.42
1:D:54:ARG:O	1:D:128:TYR:HD1	2.03	0.41
1:C:149:HIS:HA	1:C:152:VAL:HG23	2.02	0.41
1:A:61:LEU:N	1:A:62:PRO:HD2	2.35	0.41
1:A:37:TYR:CD1	1:A:155:PRO:HD3	2.56	0.41
1:C:253:ASN:HA	1:C:276:PRO:HG2	2.02	0.41
1:A:236:LEU:HD21	1:A:245:PHE:HE1	1.85	0.41
1:D:75:THR:CB	1:D:85:VAL:HG11	2.51	0.41
1:A:56:PHE:HD2	1:A:59:LEU:HD12	1.86	0.41
1:C:54:ARG:O	1:C:128:TYR:HD1	2.03	0.41
1:C:75:THR:CB	1:C:85:VAL:HG11	2.51	0.41
1:B:61:LEU:N	1:B:62:PRO:HD2	2.36	0.41
1:C:59:LEU:HD11	1:C:63:GLU:HB2	2.02	0.41
1:C:99:LYS:O	1:C:103:VAL:HG23	2.20	0.41
1:C:212:VAL:HG22	1:C:216:TYR:CB	2.51	0.41
1:D:74:LEU:CD2	1:D:117:VAL:HG11	2.51	0.41
1:A:219:HIS:CE1	1:A:274:GLN:HE22	2.39	0.40
1:B:56:PHE:HD2	1:B:59:LEU:HD12	1.85	0.40
1:D:59:LEU:HD11	1:D:63:GLU:CB	2.51	0.40
1:B:37:TYR:CD1	1:B:155:PRO:HD3	2.55	0.40
1:D:149:HIS:HA	1:D:152:VAL:HG23	2.02	0.40
1:B:30:MET:HB3	1:B:31:PHE:H	1.71	0.40
1:B:32:ASP:HA	1:B:33:PRO:HD2	1.86	0.40
1:D:52:HIS:HE1	1:D:128:TYR:O	2.04	0.40
1:D:99:LYS:O	1:D:103:VAL:HG23	2.21	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	212/299 (71%)	203 (96%)	8 (4%)	1 (0%)	24	42
1	B	219/299 (73%)	211 (96%)	7 (3%)	1 (0%)	24	42
1	C	212/299 (71%)	200 (94%)	11 (5%)	1 (0%)	24	42
1	D	212/299 (71%)	200 (94%)	10 (5%)	2 (1%)	14	28
All	All	855/1196 (72%)	814 (95%)	36 (4%)	5 (1%)	21	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	PRO
1	D	201	PRO
1	D	223	VAL
1	A	201	PRO
1	B	201	PRO

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	172/261 (66%)	163 (95%)	9 (5%)	21	43
1	B	173/261 (66%)	163 (94%)	10 (6%)	18	38
1	C	168/261 (64%)	153 (91%)	15 (9%)	9	20
1	D	164/261 (63%)	148 (90%)	16 (10%)	7	16
All	All	677/1044 (65%)	627 (93%)	50 (7%)	13	26

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	59	LEU
1	A	61	LEU
1	A	79	SER
1	A	103	VAL
1	A	163	CYS
1	A	212	VAL
1	A	255	LYS
1	A	287	HIS
1	B	51	ASN
1	B	59	LEU
1	B	60	THR
1	B	61	LEU
1	B	79	SER
1	B	103	VAL
1	B	163	CYS
1	B	212	VAL
1	B	255	LYS
1	B	287	HIS
1	C	36	LYS
1	C	74	LEU
1	C	76	ARG
1	C	110	ASP
1	C	115	VAL
1	C	142	LEU
1	C	146	ASP
1	C	199	THR
1	C	219	HIS
1	C	220	ARG
1	C	232	LEU
1	C	235	MET
1	C	243	LEU
1	C	251	LEU
1	C	286	LEU
1	D	36	LYS
1	D	41	HIS
1	D	74	LEU
1	D	76	ARG
1	D	110	ASP
1	D	115	VAL
1	D	140	THR
1	D	142	LEU

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Mol	Chain	Res	Type
1	D	146	ASP
1	D	199	THR
1	D	219	HIS
1	D	232	LEU
1	D	235	MET
1	D	243	LEU
1	D	251	LEU
1	D	286	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	51	ASN
1	A	52	HIS
1	A	89	ASN
1	A	258	GLN
1	B	41	HIS
1	B	51	ASN
1	B	52	HIS
1	B	89	ASN
1	B	258	GLN
1	B	274	GLN
1	C	52	HIS
1	C	121	HIS
1	C	219	HIS
1	C	258	GLN
1	D	52	HIS
1	D	121	HIS
1	D	219	HIS
1	D	258	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

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	219/299 (73%)	1.43	45 (20%)	2 2	13, 28, 38, 40	1 (0%)
1	B	227/299 (75%)	1.56	57 (25%)	1 1	19, 29, 38, 40	0
1	C	220/299 (73%)	1.62	53 (24%)	2 1	29, 35, 42, 44	0
1	D	220/299 (73%)	1.56	55 (25%)	2 1	29, 35, 42, 44	0
All	All	886/1196 (74%)	1.54	210 (23%)	2 2	13, 32, 40, 44	1 (0%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	PHE	6.5
1	B	292	SER	6.2
1	A	104	SER	6.1
1	B	215	GLY	5.4
1	A	105	THR	5.4
1	B	51	ASN	5.3
1	B	194	ALA	5.2
1	A	199	THR	4.9
1	D	67	THR	4.8
1	B	102	GLU	4.6
1	A	122	GLY	4.4
1	A	195	ALA	4.3
1	A	57	TRP	4.2
1	B	197	VAL	4.2
1	A	194	ALA	4.2
1	B	60	THR	4.0
1	C	149	HIS	4.0
1	D	223	VAL	3.9
1	B	219	HIS	3.9
1	C	229	ILE	3.9
1	D	222	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	223	VAL	3.8
1	A	54	ARG	3.7
1	D	111	ALA	3.7
1	A	28	ARG	3.7
1	C	62	PRO	3.6
1	A	201	PRO	3.6
1	D	217	TYR	3.6
1	B	65	ARG	3.6
1	A	111	ALA	3.5
1	A	261	VAL	3.5
1	B	199	THR	3.5
1	C	217	TYR	3.5
1	B	268	SER	3.4
1	B	58	HIS	3.4
1	B	163	CYS	3.4
1	C	69	ALA	3.4
1	B	269	ALA	3.4
1	D	69	ALA	3.4
1	A	65	ARG	3.3
1	A	29	GLU	3.3
1	D	145	GLY	3.3
1	C	244	GLU	3.3
1	D	230	GLN	3.3
1	B	122	GLY	3.3
1	B	125	ASN	3.3
1	D	59	LEU	3.3
1	C	218	SER	3.3
1	D	112	ASP	3.2
1	A	103	VAL	3.2
1	B	57	TRP	3.2
1	C	289	PHE	3.1
1	C	100	ILE	3.1
1	A	33	PRO	3.1
1	D	74	LEU	3.1
1	D	200	LEU	3.1
1	A	196	SER	3.1
1	C	101	HIS	3.1
1	D	149	HIS	3.1
1	C	109	ALA	3.0
1	C	103	VAL	3.0
1	B	123	GLU	3.0
1	C	207	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	238	LYS	3.0
1	A	106	VAL	3.0
1	B	262	ASP	3.0
1	D	237	GLY	3.0
1	B	126	HIS	3.0
1	B	198	TYR	2.9
1	C	30	MET	2.9
1	D	278	PHE	2.9
1	C	59	LEU	2.9
1	D	110	ASP	2.9
1	C	56	PHE	2.8
1	D	65	ARG	2.8
1	D	88	PHE	2.8
1	A	60	THR	2.8
1	C	257	SER	2.8
1	D	199	THR	2.8
1	D	124	GLY	2.8
1	D	57	TRP	2.8
1	A	206	PHE	2.8
1	C	88	PHE	2.8
1	B	72	ASP	2.8
1	B	103	VAL	2.7
1	B	202	ALA	2.7
1	A	163	CYS	2.7
1	C	232	LEU	2.7
1	B	110	ASP	2.7
1	B	259	ARG	2.7
1	B	222	THR	2.7
1	C	140	THR	2.7
1	C	145	GLY	2.7
1	D	224	ASN	2.7
1	D	78	PHE	2.6
1	C	57	TRP	2.6
1	A	120	SER	2.6
1	B	129	ALA	2.6
1	A	100	ILE	2.6
1	B	46	ILE	2.6
1	B	131	ASP	2.6
1	B	213	ALA	2.6
1	D	211	SER	2.6
1	B	43	ARG	2.6
1	A	138	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	32	ASP	2.6
1	B	260	ARG	2.6
1	A	59	LEU	2.5
1	B	88	PHE	2.5
1	C	40	ASP	2.5
1	B	48	LEU	2.5
1	D	54	ARG	2.5
1	D	201	PRO	2.5
1	D	85	VAL	2.5
1	A	130	TYR	2.5
1	C	199	THR	2.5
1	C	90	ASP	2.4
1	D	261	VAL	2.4
1	B	195	ALA	2.4
1	D	195	ALA	2.4
1	A	224	ASN	2.4
1	C	89	ASN	2.4
1	B	207	LEU	2.4
1	D	119	LEU	2.4
1	D	66	GLY	2.4
1	A	119	LEU	2.4
1	C	87	CYS	2.4
1	D	116	CYS	2.4
1	A	197	VAL	2.4
1	C	238	LYS	2.4
1	C	55	PHE	2.4
1	A	198	TYR	2.4
1	B	200	LEU	2.4
1	B	45	GLY	2.4
1	B	63	GLU	2.4
1	C	150	SER	2.4
1	D	216	TYR	2.4
1	B	56	PHE	2.3
1	A	219	HIS	2.3
1	C	157	ILE	2.3
1	B	85	VAL	2.3
1	C	261	VAL	2.3
1	D	64	ARG	2.3
1	D	89	ASN	2.3
1	A	277	CYS	2.3
1	C	68	CYS	2.3
1	C	49	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	117	VAL	2.3
1	B	74	LEU	2.3
1	D	142	LEU	2.3
1	D	207	LEU	2.3
1	B	128	TYR	2.3
1	B	244	GLU	2.3
1	D	132	ALA	2.3
1	C	79	SER	2.3
1	C	212	VAL	2.3
1	D	45	GLY	2.3
1	D	134	ILE	2.2
1	D	103	VAL	2.2
1	D	56	PHE	2.2
1	D	214	GLU	2.2
1	B	75	THR	2.2
1	C	163	CYS	2.2
1	B	150	SER	2.2
1	A	123	GLU	2.2
1	B	286	LEU	2.2
1	C	142	LEU	2.2
1	B	267	PRO	2.2
1	D	123	GLU	2.2
1	C	46	ILE	2.2
1	D	101	HIS	2.2
1	D	246	THR	2.2
1	A	227	TRP	2.2
1	C	237	GLY	2.2
1	D	232	LEU	2.2
1	B	204	ALA	2.2
1	C	127	ILE	2.1
1	C	73	ASN	2.1
1	B	66	GLY	2.1
1	A	260	ARG	2.1
1	A	115	VAL	2.1
1	B	118	PHE	2.1
1	D	151	LEU	2.1
1	A	43	ARG	2.1
1	A	258	GLN	2.1
1	A	51	ASN	2.1
1	C	92	LYS	2.1
1	D	225	GLY	2.1
1	D	260	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	279	ALA	2.1
1	A	216	TYR	2.1
1	A	85	VAL	2.1
1	C	91	LEU	2.1
1	C	66	GLY	2.1
1	C	118	PHE	2.1
1	C	138	THR	2.1
1	A	132	ALA	2.1
1	D	46	ILE	2.1
1	D	281	MET	2.0
1	A	71	ARG	2.0
1	A	88	PHE	2.0
1	B	54	ARG	2.0
1	C	203	GLY	2.0
1	D	227	TRP	2.0
1	B	230	GLN	2.0
1	D	62	PRO	2.0
1	C	236	LEU	2.0
1	D	289	PHE	2.0
1	A	127	ILE	2.0
1	C	106	VAL	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($\text{\AA}^2$)	Q<0.9
2	ZN	A	301	1/1	0.67	0.10	21,21,21,21	0
2	ZN	D	301	1/1	0.78	0.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	301	1/1	0.83	0.16	34,34,34,34	0
2	ZN	B	301	1/1	0.94	0.08	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.