



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:20 am GMT

PDB ID : 5C0Q
Title : Crystal structure of Zn bound CbsA from *Thermotoga neapolitana*
Authors : Ha, N.C.; Kim, J.S.; Yoon, B.Y.
Deposited on : 2015-06-12
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

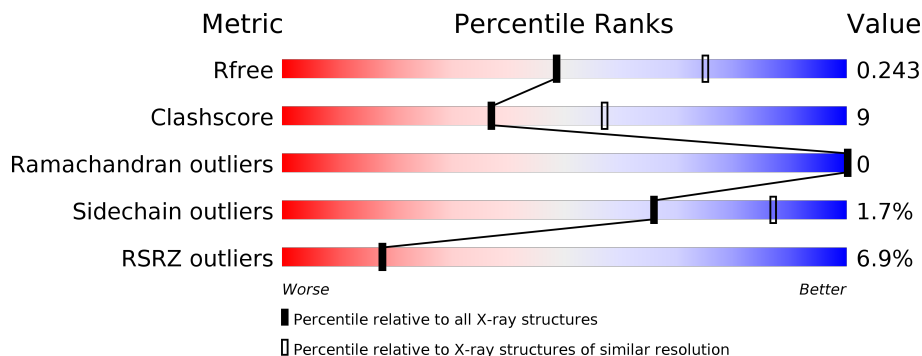
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 $\leq 5\%$. 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	467	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>• •</div> </div> </div>
1	B	467	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>• •</div> </div> </div>
1	C	467	<div> <div>13%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 6%</div> </div> </div>
1	D	467	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14208 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 Beta-N-acetylhexosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3583	2304	602	660	17			
1	B	457	Total	C	N	O	S	0	0	0
			3631	2333	610	671	17			
1	C	441	Total	C	N	O	S	0	0	0
			3516	2264	589	647	16			
1	D	434	Total	C	N	O	S	0	0	0
			3443	2223	569	636	15			

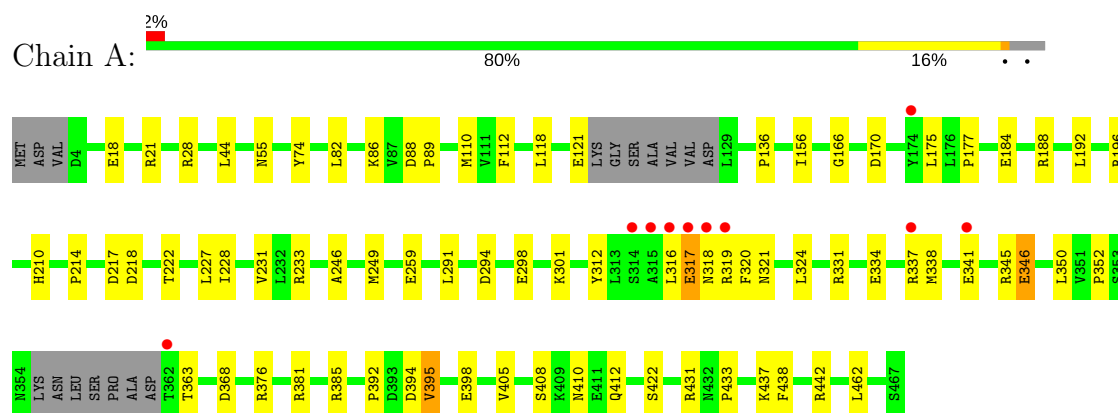
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Zn	0	0
			9	9		
2	A	10	Total	Zn	0	0
			10	10		
2	D	7	Total	Zn	0	0
			7	7		
2	C	9	Total	Zn	0	0
			9	9		

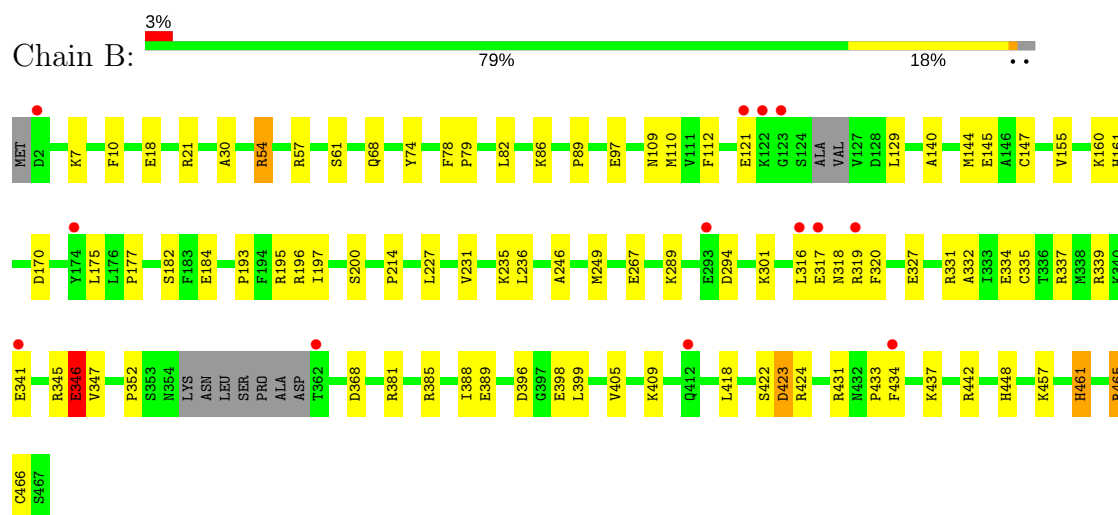
3 Residue-property plots [i](#)

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.

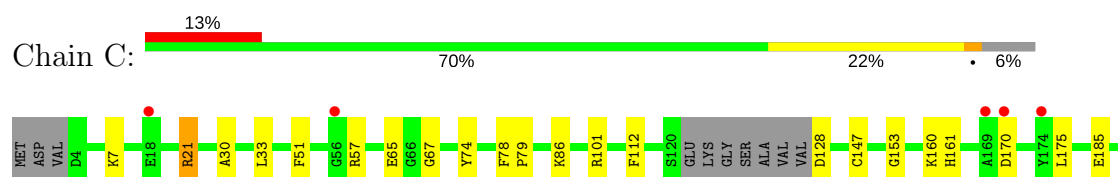
• Molecule 1: Beta-N-acetylhexosaminidase

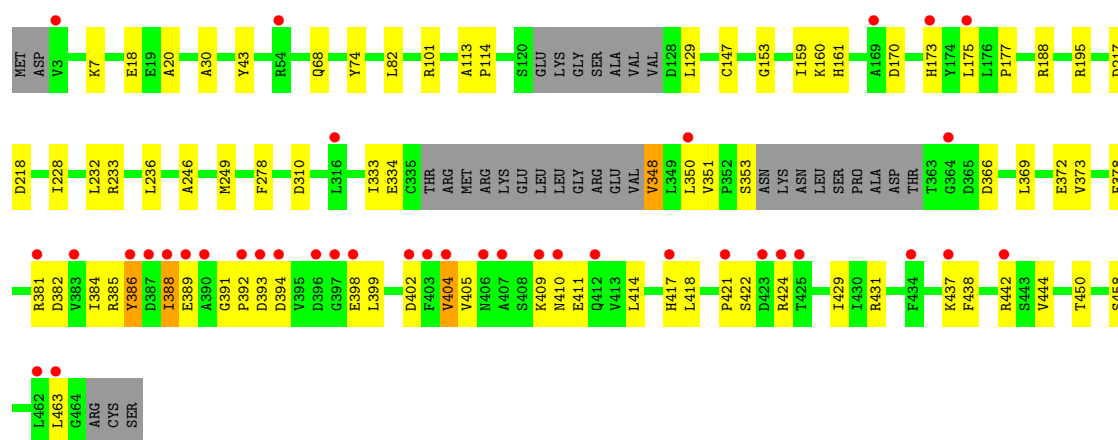


• Molecule 1: Beta-N-acetylhexosaminidase



• Molecule 1: Beta-N-acetylhexosaminidase





4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	158.84Å 158.84Å 520.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.97-2.50) 99.8 (19.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.22 (at 2.50Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.201 , 0.242 0.195 , 0.243	Depositor DCC
R_{free} test set	3951 reflections (2.34%)	DCC
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14208	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.25 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.8145e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.76	0/3660	0.75	1/4939 (0.0%)
1	B	0.80	3/3708 (0.1%)	0.78	1/5003 (0.0%)
1	C	0.62	0/3592	0.78	4/4846 (0.1%)
1	D	0.64	1/3519 (0.0%)	0.70	1/4753 (0.0%)
All	All	0.71	4/14479 (0.0%)	0.76	7/19541 (0.0%)

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	1
1	C	0	2
1	D	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	CYS	CB-SG	-6.22	1.71	1.82
1	B	335	CYS	CB-SG	-5.45	1.73	1.81
1	B	147	CYS	CB-SG	-5.04	1.73	1.81
1	B	346	GLU	CB-CG	5.00	1.61	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	397	GLY	N-CA-C	-7.82	93.55	113.10
1	C	381	ARG	CG-CD-NE	-7.00	97.10	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	D	386	TYR	N-CA-CB	-5.54	100.63	110.60
1	A	331	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	C	381	ARG	CB-CA-C	-5.33	99.74	110.40
1	C	335	CYS	CA-CB-SG	5.14	123.25	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	GLU	Peptide
1	C	339	ARG	Peptide
1	C	461	HIS	Peptide
1	D	348	VAL	Peptide
1	D	421	PRO	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	3583	0	3573	52	1
1	B	3631	0	3620	62	1
1	C	3516	0	3505	95	1
1	D	3443	0	3420	58	1
2	A	10	0	0	0	0
2	B	9	0	0	0	0
2	C	9	0	0	1	0
2	D	7	0	0	0	0
All	All	14208	0	14118	252	2

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 9.

All (252) 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:C:396:ASP:OD2	1:C:424:ARG:NH1	1.88	1.06
1:C:345:ARG:HE	1:C:399:LEU:HB2	1.31	0.94
1:C:345:ARG:NH2	1:C:398:GLU:O	2.03	0.92
1:A:437:LYS:NZ	1:B:121:GLU:OE2	2.10	0.84
1:A:121:GLU:OE2	1:B:437:LYS:NZ	2.10	0.82
1:C:345:ARG:NH2	1:C:424:ARG:HB2	1.94	0.82
1:A:334:GLU:OE2	1:B:86:LYS:NZ	2.12	0.81
1:C:327:GLU:OE1	1:C:331:ARG:NH1	2.14	0.80
1:C:347:VAL:O	1:C:381:ARG:NH2	2.13	0.80
1:C:386:TYR:OH	1:C:403:PHE:O	2.00	0.80
1:B:18:GLU:OE1	1:B:21:ARG:NH1	2.14	0.79
1:C:346:GLU:C	1:C:381:ARG:NH1	2.38	0.77
1:A:368:ASP:OD1	1:A:385:ARG:NH2	2.18	0.77
1:A:86:LYS:NZ	1:B:334:GLU:OE1	2.12	0.76
1:D:410:ASN:OD1	1:D:411:GLU:N	2.18	0.76
1:A:319:ARG:NH2	1:B:97:GLU:OE2	2.20	0.75
1:C:337:ARG:NH1	1:C:338:MET:O	2.17	0.75
1:B:368:ASP:OD1	1:B:385:ARG:NH2	2.20	0.74
1:B:422:SER:HB2	1:B:442:ARG:NH1	2.03	0.74
1:A:18:GLU:HG2	1:A:21:ARG:HH21	1.52	0.73
1:C:346:GLU:C	1:C:381:ARG:HH12	1.92	0.73
1:C:259:GLU:HG3	1:C:291:LEU:HD11	1.71	0.71
1:C:347:VAL:N	1:C:381:ARG:HH12	1.88	0.71
1:C:418:LEU:HG	1:C:442:ARG:NH1	2.05	0.71
1:B:339:ARG:NH2	1:B:423:ASP:O	2.23	0.70
1:C:347:VAL:CA	1:C:381:ARG:HH12	2.04	0.70
1:C:346:GLU:O	1:C:381:ARG:NH1	2.26	0.69
1:A:352:PRO:O	1:A:385:ARG:NH1	2.26	0.69
1:D:351:VAL:HG23	1:D:385:ARG:HH11	1.58	0.68
1:B:144:MET:HE2	1:B:197:ILE:HD13	1.77	0.67
1:B:352:PRO:O	1:B:385:ARG:NH1	2.28	0.67
1:C:378:PHE:CZ	1:C:463:LEU:HD11	2.29	0.67
1:B:109:ASN:HB2	1:B:316:LEU:HD22	1.78	0.66
1:B:144:MET:HE3	1:B:196:ARG:HG3	1.77	0.66
1:C:346:GLU:HG3	1:C:381:ARG:CZ	2.26	0.66
1:A:318:ASN:OD1	1:A:320:PHE:HB2	1.96	0.65
1:D:170:ASP:HB3	1:D:175:LEU:HD11	1.77	0.65
1:A:121:GLU:HG3	1:B:434:PHE:CD2	2.32	0.65
1:B:144:MET:HE1	1:B:197:ILE:HA	1.78	0.65
1:C:57:ARG:NH1	1:C:317:GLU:OE2	2.30	0.65
1:A:217:ASP:OD1	1:A:218:ASP:N	2.30	0.65
1:A:317:GLU:O	1:A:318:ASN:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:HD11	1:C:438:PHE:HB3	1.80	0.63
1:D:388:ILE:HD13	1:D:405:VAL:HB	1.80	0.63
1:D:386:TYR:OH	1:D:417:HIS:NE2	2.32	0.63
1:A:170:ASP:HB2	1:A:177:PRO:HB3	1.81	0.62
1:C:461:HIS:HA	1:C:464:GLY:H	1.65	0.62
1:D:398:GLU:O	1:D:424:ARG:HG2	1.99	0.62
1:C:7:LYS:HA	1:C:30:ALA:HB2	1.80	0.61
1:C:7:LYS:HE2	1:C:310:ASP:OD1	2.01	0.61
1:B:318:ASN:OD1	1:B:319:ARG:N	2.33	0.61
1:C:287:SER:O	1:C:291:LEU:HD13	2.00	0.60
1:D:404:VAL:HG22	1:D:429:ILE:HA	1.84	0.60
1:C:185:GLU:OE2	2:C:1004:ZN:ZN	1.49	0.60
1:A:422:SER:HB2	1:A:442:ARG:NH1	2.16	0.59
1:C:388:ILE:HG21	1:C:405:VAL:HB	1.84	0.59
1:A:156:ILE:HG12	1:A:316:LEU:HD21	1.85	0.59
1:D:389:GLU:OE2	1:D:409:LYS:HE3	2.03	0.59
1:A:82:LEU:HD21	1:B:433:PRO:HG3	1.85	0.58
1:D:350:LEU:HD11	1:D:384:ILE:HB	1.86	0.58
1:D:217:ASP:OD1	1:D:218:ASP:N	2.36	0.58
1:C:33:LEU:HD22	1:C:112:PHE:HE2	1.69	0.56
1:B:54:ARG:HH22	1:B:327:GLU:HG3	1.70	0.56
1:B:200:SER:HB2	1:C:200:SER:HB2	1.88	0.56
1:C:348:VAL:N	1:C:399:LEU:O	2.24	0.55
1:D:7:LYS:HE2	1:D:310:ASP:OD1	2.06	0.55
1:C:170:ASP:HB3	1:C:175:LEU:HD11	1.88	0.55
1:D:381:ARG:HD3	1:D:381:ARG:N	2.21	0.55
1:D:422:SER:HB2	1:D:442:ARG:CZ	2.37	0.55
1:C:404:VAL:HG22	1:C:429:ILE:HA	1.88	0.54
1:D:437:LYS:HG3	1:D:438:PHE:CD1	2.42	0.54
1:C:347:VAL:N	1:C:381:ARG:NH1	2.56	0.54
1:A:74:TYR:HA	1:B:74:TYR:HA	1.90	0.54
1:D:393:ASP:OD1	1:D:394:ASP:N	2.40	0.54
1:B:144:MET:CE	1:B:196:ARG:HG3	2.37	0.54
1:D:386:TYR:OH	1:D:388:ILE:HG23	2.08	0.54
1:C:400:ILE:HG12	1:C:420:LEU:HD23	1.90	0.53
1:B:110:MET:HE1	1:B:112:PHE:HE1	1.74	0.53
1:B:341:GLU:CD	1:B:341:GLU:H	2.10	0.53
1:C:437:LYS:HG3	1:C:438:PHE:CD1	2.43	0.53
1:C:290:LYS:O	1:C:294:ASP:HB3	2.10	0.52
1:A:156:ILE:CG1	1:A:316:LEU:HD21	2.39	0.52
1:C:346:GLU:O	1:C:398:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLU:OE1	1:A:301:LYS:NZ	2.30	0.52
1:B:405:VAL:HG22	1:B:431:ARG:HG3	1.91	0.52
1:C:420:LEU:O	1:C:442:ARG:NH2	2.43	0.52
1:C:342:LEU:O	1:C:345:ARG:HB3	2.09	0.52
1:C:78:PHE:CD1	1:C:79:PRO:HD2	2.44	0.52
1:C:257:SER:H	1:C:260:GLU:HG3	1.75	0.51
1:C:421:PRO:HB2	1:C:424:ARG:HE	1.75	0.51
1:D:378:PHE:CE1	1:D:463:LEU:HD21	2.46	0.51
1:A:184:GLU:OE2	1:A:188:ARG:NH1	2.43	0.51
1:C:399:LEU:HD12	1:C:400:ILE:N	2.26	0.51
1:C:392:PRO:HD3	1:C:417:HIS:CE1	2.46	0.51
1:B:231:VAL:HA	1:B:235:LYS:HG3	1.92	0.51
1:B:339:ARG:HB3	1:B:341:GLU:OE2	2.11	0.51
1:C:226:LYS:HD2	1:C:230:GLU:HB2	1.92	0.51
1:A:136:PRO:HB2	1:A:192:LEU:HD23	1.93	0.50
1:B:418:LEU:O	1:B:442:ARG:NH2	2.44	0.50
1:C:427:TYR:HB2	1:C:444:VAL:HG22	1.93	0.50
1:C:257:SER:OG	1:C:260:GLU:HG2	2.10	0.50
1:D:411:GLU:HG3	1:D:411:GLU:O	2.12	0.50
1:D:333:ILE:HD13	1:D:458:SER:HA	1.94	0.50
1:C:345:ARG:NE	1:C:399:LEU:HB2	2.14	0.50
1:A:259:GLU:HG3	1:A:291:LEU:HD21	1.93	0.49
1:B:110:MET:CE	1:B:112:PHE:HE1	2.24	0.49
1:C:128:ASP:OD2	1:D:431:ARG:NH1	2.44	0.49
1:B:461:HIS:CD2	1:B:465:ARG:HD3	2.47	0.49
1:A:44:LEU:HD11	1:A:376:ARG:NH2	2.26	0.49
1:C:340:LYS:HB3	1:C:341:GLU:OE1	2.11	0.49
1:A:317:GLU:HG2	1:A:318:ASN:N	2.27	0.49
1:C:21:ARG:HG3	1:C:51:PHE:CZ	2.47	0.49
1:B:195:ARG:HG2	1:B:236:LEU:CD2	2.42	0.49
1:B:57:ARG:NH2	1:B:317:GLU:H	2.11	0.49
1:B:327:GLU:OE1	1:B:331:ARG:HD2	2.12	0.49
1:C:345:ARG:CZ	1:C:398:GLU:O	2.60	0.49
1:A:346:GLU:CD	1:A:381:ARG:HH21	2.15	0.48
1:A:410:ASN:OD1	1:A:412:GLN:N	2.43	0.48
1:C:415:GLN:O	1:C:415:GLN:HG3	2.12	0.48
1:B:345:ARG:HD3	1:B:398:GLU:HB3	1.95	0.48
1:A:312:TYR:O	1:A:316:LEU:HG	2.14	0.48
1:B:396:ASP:CG	1:B:424:ARG:HH21	2.17	0.48
1:C:341:GLU:C	1:C:343:LEU:H	2.13	0.48
1:C:414:LEU:HG	1:C:414:LEU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ARG:HD3	1:A:398:GLU:HB3	1.96	0.47
1:C:347:VAL:C	1:C:381:ARG:HH22	2.14	0.47
1:C:347:VAL:HG11	1:C:401:PHE:CD2	2.48	0.47
1:B:175:LEU:O	1:B:177:PRO:HD3	2.13	0.47
1:C:433:PRO:HG3	1:D:82:LEU:HD21	1.96	0.47
1:B:347:VAL:HG22	1:B:399:LEU:HD23	1.96	0.47
1:B:68:GLN:OE1	1:B:129:LEU:HB2	2.14	0.47
1:D:228:ILE:O	1:D:233:ARG:HG2	2.15	0.47
1:B:170:ASP:HB3	1:B:175:LEU:HD11	1.96	0.47
1:D:404:VAL:HG21	1:D:429:ILE:HG13	1.96	0.47
1:D:246:ALA:HB3	1:D:249:MET:HE2	1.96	0.47
1:C:392:PRO:CD	1:C:417:HIS:ND1	2.77	0.47
1:D:429:ILE:HD13	1:D:444:VAL:HG13	1.97	0.47
1:C:345:ARG:HH22	1:C:424:ARG:HB2	1.72	0.47
1:C:74:TYR:HA	1:D:74:TYR:HA	1.97	0.47
1:C:257:SER:H	1:C:260:GLU:CG	2.29	0.46
1:C:307:LYS:NZ	1:C:311:GLU:OE2	2.47	0.46
1:D:348:VAL:N	1:D:399:LEU:O	2.48	0.46
1:D:405:VAL:HG22	1:D:431:ARG:HG3	1.96	0.46
1:C:228:ILE:O	1:C:233:ARG:HG2	2.15	0.46
1:A:338:MET:HG3	1:A:462:LEU:HD12	1.96	0.46
1:B:78:PHE:CD1	1:B:79:PRO:HD2	2.51	0.46
1:A:433:PRO:HG3	1:B:82:LEU:HD21	1.97	0.46
1:C:290:LYS:NZ	1:C:290:LYS:HB2	2.30	0.46
1:C:340:LYS:HB2	1:C:340:LYS:HE3	1.69	0.46
1:A:28:ARG:NH1	1:A:55:ASN:O	2.48	0.46
1:A:394:ASP:OD1	1:A:395:VAL:N	2.49	0.46
1:B:294:ASP:C	1:B:294:ASP:OD1	2.53	0.46
1:C:437:LYS:HE3	1:C:438:PHE:CE1	2.50	0.46
1:C:209:ALA:O	1:C:221:ALA:HB3	2.16	0.45
1:C:246:ALA:HB3	1:C:249:MET:HE2	1.97	0.45
1:C:387:ASP:OD1	1:C:389:GLU:HG2	2.16	0.45
1:A:319:ARG:CZ	1:B:97:GLU:OE2	2.64	0.45
1:B:170:ASP:HB2	1:B:177:PRO:HB3	1.98	0.45
1:B:89:PRO:HB2	1:B:145:GLU:HG3	1.98	0.45
1:C:160:LYS:HA	1:C:161:HIS:HA	1.79	0.45
1:C:394:ASP:OD1	1:C:395:VAL:N	2.50	0.45
1:A:294:ASP:C	1:A:294:ASP:OD1	2.56	0.45
1:A:196:ARG:HA	1:A:196:ARG:HD3	1.79	0.44
1:B:160:LYS:HA	1:B:161:HIS:HA	1.83	0.44
1:C:346:GLU:CG	1:C:381:ARG:CZ	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:399:LEU:HD12	1:C:400:ILE:H	1.81	0.44
1:D:348:VAL:CG1	1:D:381:ARG:H	2.30	0.44
1:A:110:MET:CE	1:A:112:PHE:HE1	2.31	0.44
1:A:408:SER:HG	1:A:438:PHE:HE2	1.62	0.44
1:C:461:HIS:HA	1:C:464:GLY:N	2.30	0.44
1:D:173:HIS:HA	1:D:249:MET:HG2	1.99	0.44
1:B:346:GLU:CD	1:B:381:ARG:HH21	2.18	0.44
1:D:386:TYR:OH	1:D:392:PRO:HD3	2.18	0.44
1:A:405:VAL:HG22	1:A:431:ARG:HG3	1.99	0.44
1:B:318:ASN:HD21	1:B:320:PHE:HB2	1.81	0.44
1:B:389:GLU:HB3	1:B:409:LYS:NZ	2.32	0.44
1:B:461:HIS:HB3	1:B:466:CYS:SG	2.57	0.44
1:D:114:PRO:HD2	1:D:159:ILE:HG22	1.99	0.44
1:D:414:LEU:HD11	1:D:438:PHE:HB3	2.00	0.44
1:C:86:LYS:NZ	1:D:334:GLU:OE2	2.24	0.43
1:A:321:ASN:O	1:A:324:LEU:HD23	2.19	0.43
1:D:175:LEU:O	1:D:177:PRO:HD3	2.17	0.43
1:A:246:ALA:HB3	1:A:249:MET:HE2	2.01	0.43
1:B:267:GLU:OE1	1:B:301:LYS:NZ	2.52	0.43
1:B:289:LYS:HB3	1:B:289:LYS:HE2	1.60	0.43
1:A:341:GLU:CD	1:A:341:GLU:H	2.22	0.43
1:D:442:ARG:HD3	1:D:442:ARG:HA	1.82	0.43
1:A:437:LYS:HG3	1:A:438:PHE:CD1	2.53	0.43
1:D:101:ARG:HA	1:D:153:GLY:O	2.18	0.43
1:C:411:GLU:HG3	1:C:411:GLU:O	2.18	0.43
1:D:402:ASP:OD2	1:D:417:HIS:ND1	2.35	0.43
1:B:388:ILE:HG13	1:B:389:GLU:HG3	2.01	0.42
1:D:437:LYS:HE3	1:D:438:PHE:CE1	2.54	0.42
1:A:227:LEU:O	1:A:231:VAL:HB	2.19	0.42
1:C:212:LYS:HD2	1:C:218:ASP:O	2.19	0.42
1:D:351:VAL:CG2	1:D:385:ARG:HH11	2.29	0.42
1:A:228:ILE:O	1:A:233:ARG:HG2	2.20	0.42
1:A:118:LEU:O	1:A:166:GLY:HA3	2.19	0.42
1:B:337:ARG:HA	1:B:337:ARG:HD2	1.85	0.42
1:C:389:GLU:HG2	1:C:389:GLU:H	1.64	0.42
1:D:348:VAL:HG11	1:D:381:ARG:H	1.85	0.42
1:C:378:PHE:HZ	1:C:463:LEU:HD11	1.81	0.42
1:D:246:ALA:O	1:D:249:MET:HB2	2.19	0.42
1:C:298:GLU:HG2	1:C:300:GLY:H	1.85	0.42
1:C:381:ARG:N	1:C:381:ARG:HH21	2.18	0.42
1:C:459:PHE:O	1:C:463:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:VAL:O	1:C:400:ILE:HA	2.19	0.42
1:D:369:LEU:O	1:D:373:VAL:HG23	2.20	0.42
1:A:210:HIS:HE1	1:A:222:THR:HG21	1.85	0.41
1:D:228:ILE:O	1:D:232:LEU:HB3	2.20	0.41
1:D:20:ALA:HA	1:D:278:PHE:CE2	2.55	0.41
1:C:341:GLU:C	1:C:343:LEU:N	2.73	0.41
1:D:7:LYS:HA	1:D:30:ALA:HB2	2.01	0.41
1:D:404:VAL:CG2	1:D:429:ILE:HG13	2.50	0.41
1:D:366:ASP:HB3	1:D:450:THR:O	2.20	0.41
1:A:437:LYS:HE2	1:A:438:PHE:CZ	2.55	0.41
1:B:246:ALA:HB3	1:B:249:MET:HE2	2.02	0.41
1:B:7:LYS:HA	1:B:30:ALA:HB2	2.01	0.41
1:C:279:ARG:O	1:C:282:PRO:HD2	2.21	0.41
1:C:65:GLU:OE2	1:C:160:LYS:NZ	2.49	0.41
1:C:67:GLY:HA2	1:C:78:PHE:O	2.20	0.41
1:C:418:LEU:O	1:C:418:LEU:HD23	2.20	0.41
1:C:331:ARG:HH11	1:C:331:ARG:HD2	1.69	0.41
1:D:160:LYS:HA	1:D:161:HIS:HA	1.80	0.41
1:B:61:SER:HA	1:B:110:MET:O	2.21	0.41
1:B:140:ALA:HA	1:B:193:PRO:HB3	2.03	0.41
1:C:101:ARG:HA	1:C:153:GLY:O	2.21	0.41
1:D:353:SER:O	1:D:353:SER:OG	2.35	0.41
1:D:43:TYR:OH	1:D:372:GLU:OE2	2.32	0.41
1:A:175:LEU:O	1:A:177:PRO:HD3	2.21	0.41
1:A:350:LEU:HD13	1:A:392:PRO:HB3	2.03	0.41
1:B:227:LEU:O	1:B:231:VAL:HB	2.20	0.41
1:B:457:LYS:HD3	1:B:457:LYS:HA	1.93	0.41
1:C:335:CYS:HB3	1:C:336:THR:O	2.21	0.41
1:D:113:ALA:HB1	1:D:114:PRO:HA	2.02	0.41
1:D:414:LEU:O	1:D:418:LEU:HD12	2.21	0.41
1:C:147:CYS:HB3	1:C:202:VAL:HG11	2.03	0.41
1:A:249:MET:HB2	1:A:249:MET:HE2	1.78	0.41
1:B:182:SER:OG	1:B:184:GLU:HG3	2.20	0.41
1:B:332:ALA:O	1:B:448:HIS:ND1	2.43	0.41
1:B:346:GLU:OE1	1:B:381:ARG:NH2	2.33	0.41
1:D:195:ARG:HG2	1:D:236:LEU:CD2	2.51	0.41
1:D:386:TYR:HE1	1:D:391:GLY:C	2.24	0.41
1:D:386:TYR:OH	1:D:417:HIS:CE1	2.74	0.41
1:D:378:PHE:HE1	1:D:463:LEU:HD21	1.86	0.41
1:C:366:ASP:HB3	1:C:450:THR:O	2.21	0.40
1:C:207:MET:HA	1:C:243:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ALA:HA	1:C:274:LEU:O	2.22	0.40
1:A:408:SER:OG	1:A:438:PHE:HE2	2.05	0.40
1:A:88:ASP:HA	1:A:89:PRO:HD2	1.93	0.40
1:C:312:TYR:O	1:C:316:LEU:HG	2.22	0.40
1:D:68:GLN:OE1	1:D:129:LEU:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:PRO:O	1:C:188:ARG:NH1[18_655]	1.84	0.36
1:A:214:PRO:O	1:D:188:ARG:NH1[4_556]	1.95	0.25

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	444/467 (95%)	429 (97%)	15 (3%)	0	100	100
1	B	451/467 (97%)	437 (97%)	14 (3%)	0	100	100
1	C	435/467 (93%)	422 (97%)	13 (3%)	0	100	100
1	D	426/467 (91%)	415 (97%)	11 (3%)	0	100	100
All	All	1756/1868 (94%)	1703 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	392/406 (97%)	388 (99%)	4 (1%)	80	93
1	B	398/406 (98%)	392 (98%)	6 (2%)	70	89
1	C	383/406 (94%)	371 (97%)	12 (3%)	45	73
1	D	376/406 (93%)	372 (99%)	4 (1%)	78	92
All	All	1549/1624 (95%)	1523 (98%)	26 (2%)	66	87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	ARG
1	A	346	GLU
1	A	363	THR
1	A	395	VAL
1	B	10	PHE
1	B	155	VAL
1	B	346	GLU
1	B	423	ASP
1	B	461	HIS
1	B	465	ARG
1	C	21	ARG
1	C	294	ASP
1	C	319	ARG
1	C	345	ARG
1	C	381	ARG
1	C	389	GLU
1	C	404	VAL
1	C	410	ASN
1	C	412	GLN
1	C	414	LEU
1	C	415	GLN
1	C	417	HIS
1	D	18	GLU
1	D	382	ASP
1	D	388	ILE
1	D	404	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	HIS
1	B	415	GLN
1	B	461	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 35 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	450/467 (96%)	-0.27	10 (2%) 62 64	13, 24, 46, 77	0
1	B	457/467 (97%)	-0.26	13 (2%) 53 56	11, 21, 50, 76	0
1	C	441/467 (94%)	0.46	61 (13%) 3 3	15, 40, 103, 128	0
1	D	434/467 (92%)	0.21	39 (8%) 10 10	16, 34, 90, 108	0
All	All	1782/1868 (95%)	0.03	123 (6%) 18 18	11, 28, 83, 128	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	6.4
1	C	381	ARG	6.4
1	C	337	ARG	6.0
1	D	390	ALA	5.0
1	C	398	GLU	5.0
1	D	386	TYR	4.9
1	D	392	PRO	4.9
1	C	341	GLU	4.9
1	C	340	LYS	4.8
1	C	404	VAL	4.7
1	C	342	LEU	4.6
1	C	412	GLN	4.5
1	D	421	PRO	4.5
1	C	293	GLU	4.5
1	D	404	VAL	4.3
1	C	402	ASP	4.2
1	B	316	LEU	4.2
1	D	389	GLU	4.2
1	C	424	ARG	4.1
1	C	295	GLY	4.1
1	C	169	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	3	VAL	3.9
1	D	424	ARG	3.8
1	C	346	GLU	3.6
1	D	364	GLY	3.6
1	C	428	PHE	3.6
1	D	397	GLY	3.5
1	D	410	ASN	3.5
1	C	401	PHE	3.4
1	C	338	MET	3.4
1	C	423	ASP	3.3
1	D	423	ASP	3.3
1	C	440	PRO	3.3
1	C	395	VAL	3.3
1	C	339	ARG	3.3
1	C	407	ALA	3.3
1	C	464	GLY	3.3
1	C	392	PRO	3.2
1	D	462	LEU	3.2
1	C	336	THR	3.2
1	D	396	ASP	3.2
1	C	386	TYR	3.1
1	D	403	PHE	3.1
1	B	122	LYS	3.1
1	D	381	ARG	3.0
1	B	362	THR	3.0
1	D	388	ILE	3.0
1	C	418	LEU	3.0
1	C	174	TYR	3.0
1	C	399	LEU	3.0
1	D	406	ASN	3.0
1	A	341	GLU	3.0
1	A	317	GLU	2.9
1	C	400	ILE	2.9
1	C	441	GLY	2.9
1	D	387	ASP	2.9
1	D	417	HIS	2.8
1	D	169	ALA	2.8
1	D	393	ASP	2.8
1	C	384	ILE	2.8
1	C	388	ILE	2.8
1	D	383	VAL	2.8
1	C	427	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	412	GLN	2.8
1	C	319	ARG	2.7
1	A	319	ARG	2.7
1	B	317	GLU	2.7
1	C	304	ARG	2.7
1	C	438	PHE	2.7
1	C	411	GLU	2.7
1	C	364	GLY	2.6
1	B	319	ARG	2.6
1	C	409	LYS	2.6
1	C	403	PHE	2.6
1	A	316	LEU	2.6
1	D	394	ASP	2.6
1	D	350	LEU	2.6
1	C	390	ALA	2.5
1	C	396	ASP	2.5
1	D	402	ASP	2.5
1	C	410	ASN	2.5
1	B	174	TYR	2.5
1	B	341	GLU	2.5
1	D	442	ARG	2.5
1	C	439	PHE	2.5
1	C	379	LYS	2.4
1	C	253	SER	2.4
1	D	434	PHE	2.4
1	C	294	ASP	2.4
1	C	314	SER	2.4
1	D	409	LYS	2.4
1	C	170	ASP	2.4
1	C	18	GLU	2.4
1	B	121	GLU	2.4
1	C	393	ASP	2.3
1	D	316	LEU	2.3
1	A	315	ALA	2.3
1	C	367	TYR	2.3
1	A	318	ASN	2.3
1	B	123	GLY	2.3
1	C	426	ILE	2.3
1	C	406	ASN	2.3
1	D	173	HIS	2.3
1	D	425	THR	2.2
1	A	337	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	2	ASP	2.2
1	C	56	GLY	2.2
1	D	398	GLU	2.2
1	C	394	ASP	2.2
1	B	434	PHE	2.2
1	C	317	GLU	2.1
1	B	293	GLU	2.1
1	A	314	SER	2.1
1	D	407	ALA	2.1
1	D	463	LEU	2.1
1	C	318	ASN	2.1
1	D	54	ARG	2.1
1	A	174	TYR	2.0
1	B	412	GLN	2.0
1	D	175	LEU	2.0
1	C	397	GLY	2.0
1	D	437	LYS	2.0
1	A	362	THR	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 carbohydrates 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. 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	B	1007	1/1	0.82	0.17	-	103,103,103,103	0
2	ZN	D	503	1/1	0.99	0.03	-	33,33,33,33	0
2	ZN	B	1008	1/1	0.95	0.10	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	A	1006	1/1	0.94	0.03	-	49,49,49,49	0
2	ZN	C	1002	1/1	0.95	0.04	-	53,53,53,53	0
2	ZN	C	1007	1/1	0.93	0.32	-	131,131,131,131	0
2	ZN	C	1004	1/1	0.98	0.05	-	29,29,29,29	0
2	ZN	B	1001	1/1	0.92	0.06	-	45,45,45,45	0
2	ZN	A	1001	1/1	0.94	0.04	-	52,52,52,52	0
2	ZN	D	505	1/1	0.93	0.28	-	109,109,109,109	0
2	ZN	D	506	1/1	0.79	0.23	-	127,127,127,127	0
2	ZN	C	1001	1/1	0.98	0.02	-	62,62,62,62	0
2	ZN	C	1006	1/1	0.52	0.22	-	103,103,103,103	0
2	ZN	A	1003	1/1	0.88	0.07	-	70,70,70,70	0
2	ZN	D	502	1/1	0.96	0.11	-	71,71,71,71	0
2	ZN	A	1007	1/1	0.95	0.07	-	71,71,71,71	0
2	ZN	A	1005	1/1	0.98	0.14	-	21,21,21,21	0
2	ZN	D	504	1/1	0.95	0.05	-	65,65,65,65	0
2	ZN	C	1005	1/1	0.98	0.08	-	70,70,70,70	0
2	ZN	A	1009	1/1	0.69	0.30	-	126,126,126,126	0
2	ZN	C	1009	1/1	0.98	0.05	-	56,56,56,56	0
2	ZN	B	1002	1/1	0.98	0.09	-	66,66,66,66	0
2	ZN	D	507	1/1	0.91	0.13	-	102,102,102,102	0
2	ZN	B	1006	1/1	0.94	0.06	-	69,69,69,69	0
2	ZN	C	1008	1/1	0.94	0.09	-	86,86,86,86	0
2	ZN	A	1004	1/1	0.93	0.05	-	60,60,60,60	0
2	ZN	B	1005	1/1	0.99	0.16	-	25,25,25,25	0
2	ZN	A	1008	1/1	0.73	0.16	-	90,90,90,90	0
2	ZN	A	1002	1/1	0.98	0.10	-	78,78,78,78	0
2	ZN	D	501	1/1	0.96	0.06	-	59,59,59,59	0
2	ZN	B	1004	1/1	0.96	0.05	-	63,63,63,63	0
2	ZN	C	1003	1/1	0.98	0.11	-	70,70,70,70	0
2	ZN	A	1010	1/1	0.95	0.07	-	48,48,48,48	0
2	ZN	B	1003	1/1	0.70	0.09	-	78,78,78,78	0
2	ZN	B	1009	1/1	0.57	0.14	-	88,88,88,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.