Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:49 am BST

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

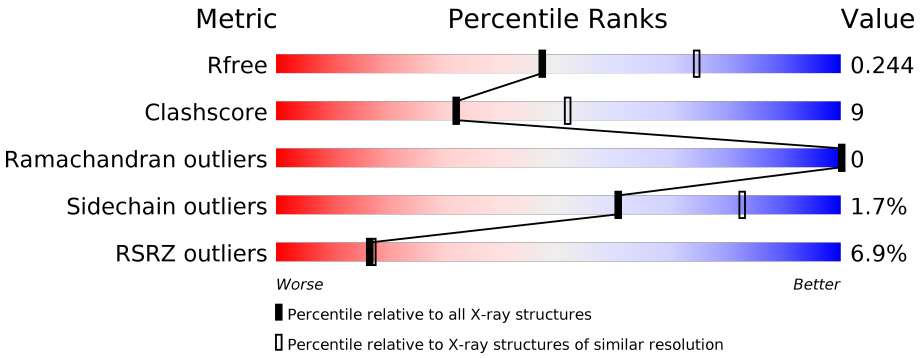
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 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 <=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	2% 80% 16%
1	B	467	3% 79% 18%
1	C	467	13% 70% 22% 6%
1	D	467	8% 76% 16% 7%

2 Entry composition (i)

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).

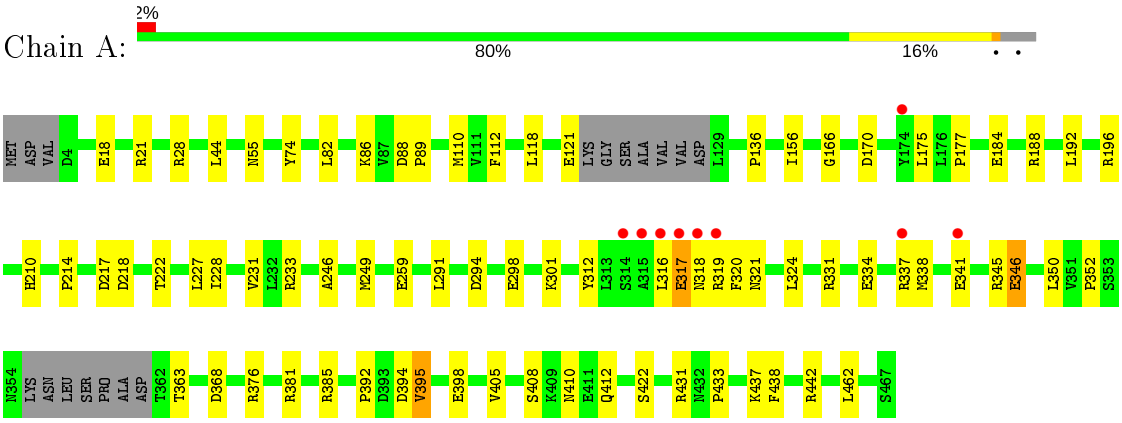
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	9	Total	Zn	0	0
			9	9		
2	A	10	Total	Zn	0	0
			10	10		
2	D	7	Total	Zn	0	0
			7	7		
2	C	9	Total	Zn	0	0
			9	9		

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.

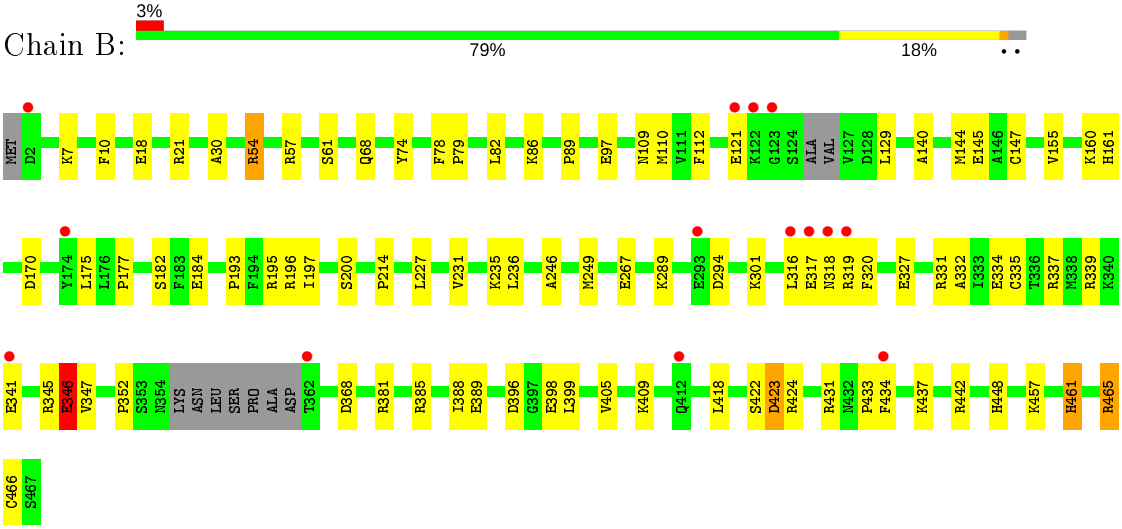
- Molecule 1: Beta-N-acetylhexosaminidase

Chain A:



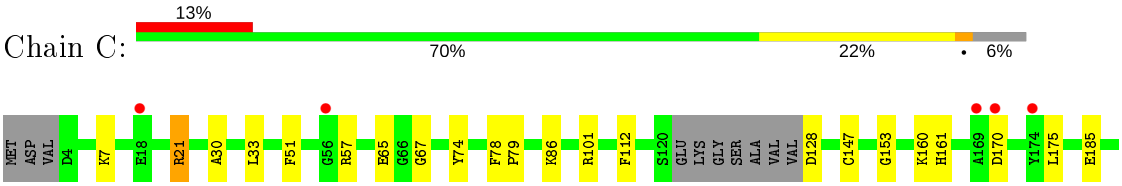
- Molecule 1: Beta-N-acetylhexosaminidase

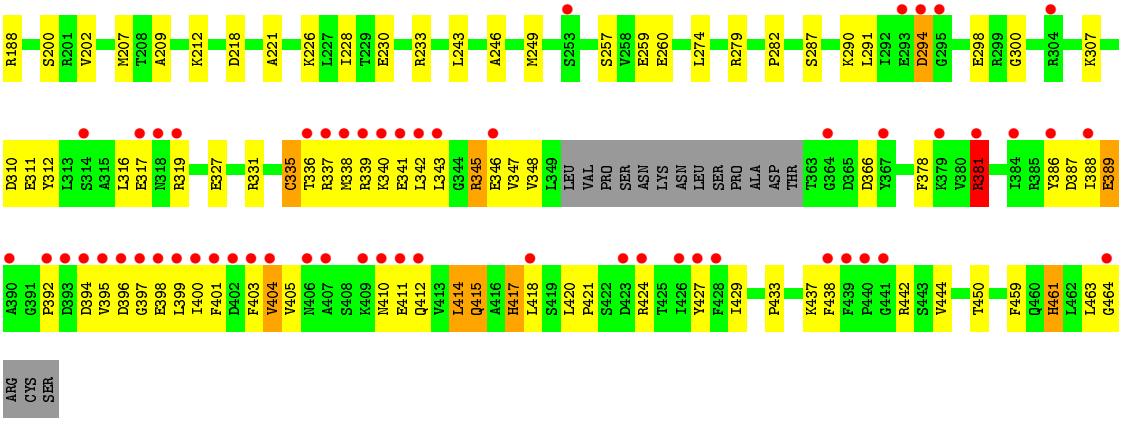
Chain B:



- Molecule 1: Beta-N-acetylhexosaminidase

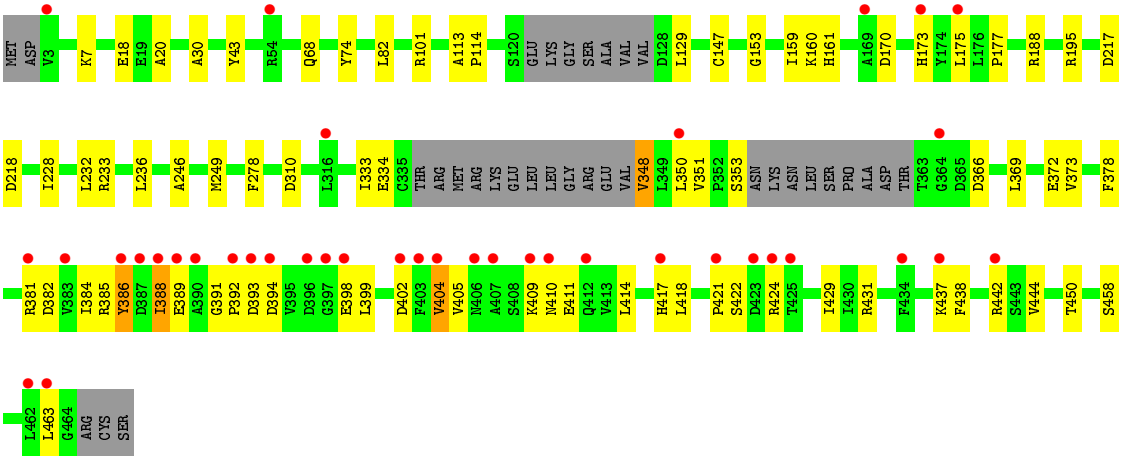
Chain C:





- Molecule 1: Beta-N-acetylhexosaminidase

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	6.01 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.201 , 0.242 0.201 , 0.244	Depositor DCC
R_{free} test set	1998 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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 2.8125e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (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	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%)	76 90
1	B	398/406 (98%)	392 (98%)	6 (2%)	65 85
1	C	383/406 (94%)	371 (97%)	12 (3%)	40 67
1	D	376/406 (93%)	372 (99%)	4 (1%)	73 89
All	All	1549/1624 (95%)	1523 (98%)	26 (2%)	60 82

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

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 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

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, 95^{th} 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	9 (2%) 65 68	13, 24, 46, 77	0
1	B	457/467 (97%)	-0.26	14 (3%) 49 52	11, 21, 50, 76	0
1	C	441/467 (94%)	0.46	61 (13%) 2 2	15, 40, 103, 128	0
1	D	434/467 (92%)	0.21	39 (8%) 9 9	16, 34, 90, 108	0
All	All	1782/1868 (95%)	0.03	123 (6%) 16 17	11, 28, 83, 128	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	343	LEU	6.5
1	C	381	ARG	6.4
1	C	337	ARG	5.8
1	C	398	GLU	5.0
1	C	341	GLU	5.0
1	D	390	ALA	4.9
1	D	386	TYR	4.9
1	C	340	LYS	4.9
1	D	392	PRO	4.9
1	C	404	VAL	4.7
1	C	342	LEU	4.7
1	C	293	GLU	4.6
1	D	421	PRO	4.6
1	C	412	GLN	4.5
1	D	404	VAL	4.4
1	C	295	GLY	4.3
1	C	402	ASP	4.2
1	C	424	ARG	4.2
1	B	316	LEU	4.2
1	D	389	GLU	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	D	364	GLY	3.7
1	C	346	GLU	3.6
1	D	397	GLY	3.6
1	C	428	PHE	3.5
1	D	410	ASN	3.5
1	C	338	MET	3.5
1	C	401	PHE	3.4
1	C	440	PRO	3.4
1	D	423	ASP	3.4
1	C	407	ALA	3.3
1	C	395	VAL	3.3
1	C	423	ASP	3.3
1	C	339	ARG	3.3
1	C	392	PRO	3.3
1	D	396	ASP	3.3
1	D	462	LEU	3.2
1	C	336	THR	3.2
1	C	464	GLY	3.2
1	D	403	PHE	3.1
1	D	381	ARG	3.0
1	C	386	TYR	3.0
1	D	388	ILE	3.0
1	D	406	ASN	3.0
1	B	122	LYS	3.0
1	B	362	THR	3.0
1	A	341	GLU	3.0
1	D	387	ASP	3.0
1	C	399	LEU	3.0
1	C	400	ILE	3.0
1	C	174	TYR	3.0
1	C	418	LEU	2.9
1	A	317	GLU	2.9
1	C	388	ILE	2.9
1	C	441	GLY	2.9
1	D	169	ALA	2.9
1	D	383	VAL	2.8
1	D	417	HIS	2.8
1	D	393	ASP	2.8
1	C	384	ILE	2.8
1	C	427	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	319	ARG	2.7
1	C	304	ARG	2.7
1	C	319	ARG	2.7
1	B	317	GLU	2.7
1	C	438	PHE	2.7
1	C	411	GLU	2.6
1	B	319	ARG	2.6
1	C	364	GLY	2.6
1	C	409	LYS	2.6
1	D	412	GLN	2.6
1	C	403	PHE	2.6
1	A	316	LEU	2.6
1	D	394	ASP	2.6
1	D	350	LEU	2.5
1	C	390	ALA	2.5
1	C	410	ASN	2.5
1	C	294	ASP	2.5
1	C	396	ASP	2.5
1	C	253	SER	2.5
1	B	341	GLU	2.5
1	D	442	ARG	2.5
1	D	402	ASP	2.5
1	C	18	GLU	2.5
1	C	314	SER	2.5
1	C	379	LYS	2.5
1	C	439	PHE	2.5
1	B	174	TYR	2.4
1	C	170	ASP	2.4
1	D	434	PHE	2.4
1	D	409	LYS	2.4
1	B	121	GLU	2.3
1	B	123	GLY	2.3
1	C	393	ASP	2.3
1	A	315	ALA	2.3
1	C	367	TYR	2.3
1	C	406	ASN	2.3
1	A	337	ARG	2.3
1	D	398	GLU	2.3
1	D	425	THR	2.3
1	D	316	LEU	2.3
1	A	318	ASN	2.3
1	C	426	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	56	GLY	2.2
1	D	173	HIS	2.2
1	B	2	ASP	2.2
1	B	434	PHE	2.2
1	B	293	GLU	2.2
1	C	317	GLU	2.2
1	C	397	GLY	2.2
1	C	394	ASP	2.1
1	D	407	ALA	2.1
1	D	463	LEU	2.1
1	C	318	ASN	2.1
1	A	314	SER	2.1
1	D	54	ARG	2.1
1	A	174	TYR	2.0
1	D	437	LYS	2.0
1	B	412	GLN	2.0
1	B	318	ASN	2.0
1	D	175	LEU	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	1006	1/1	0.53	0.22	103,103,103,103	0
2	ZN	B	1009	1/1	0.58	0.14	88,88,88,88	0
2	ZN	A	1009	1/1	0.69	0.30	126,126,126,126	0
2	ZN	B	1003	1/1	0.70	0.09	78,78,78,78	0
2	ZN	A	1008	1/1	0.73	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	D	506	1/1	0.79	0.23	127,127,127,127	0
2	ZN	B	1007	1/1	0.82	0.17	103,103,103,103	0
2	ZN	A	1003	1/1	0.88	0.07	70,70,70,70	0
2	ZN	D	507	1/1	0.91	0.12	102,102,102,102	0
2	ZN	B	1001	1/1	0.92	0.06	45,45,45,45	0
2	ZN	D	505	1/1	0.93	0.29	109,109,109,109	0
2	ZN	C	1007	1/1	0.93	0.33	131,131,131,131	0
2	ZN	A	1004	1/1	0.93	0.05	60,60,60,60	0
2	ZN	A	1006	1/1	0.94	0.03	49,49,49,49	0
2	ZN	A	1001	1/1	0.94	0.04	52,52,52,52	0
2	ZN	B	1006	1/1	0.94	0.05	69,69,69,69	0
2	ZN	C	1008	1/1	0.94	0.09	86,86,86,86	0
2	ZN	C	1002	1/1	0.95	0.04	53,53,53,53	0
2	ZN	B	1008	1/1	0.95	0.11	100,100,100,100	0
2	ZN	A	1010	1/1	0.95	0.07	48,48,48,48	0
2	ZN	D	502	1/1	0.95	0.10	71,71,71,71	0
2	ZN	D	504	1/1	0.95	0.05	65,65,65,65	0
2	ZN	A	1007	1/1	0.96	0.07	71,71,71,71	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	1009	1/1	0.98	0.05	56,56,56,56	0
2	ZN	A	1002	1/1	0.98	0.09	78,78,78,78	0
2	ZN	B	1002	1/1	0.98	0.09	66,66,66,66	0
2	ZN	A	1005	1/1	0.98	0.14	21,21,21,21	0
2	ZN	C	1004	1/1	0.98	0.05	29,29,29,29	0
2	ZN	C	1005	1/1	0.98	0.08	70,70,70,70	0
2	ZN	C	1001	1/1	0.98	0.02	62,62,62,62	0
2	ZN	D	503	1/1	0.99	0.03	33,33,33,33	0
2	ZN	B	1005	1/1	0.99	0.16	25,25,25,25	0
2	ZN	C	1003	1/1	0.99	0.11	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.