



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:28 AM UTC

PDB ID : 2Q6E / pdb_00002q6e
Title : Crystal structure of glucuronate isomerase from *Bacillus halodurans* complexed with Zn
Authors : Fedorov, A.A.; Fedorov, E.V.; Patskovsky, Y.; Toro, R.; Sauder, J.M.; Bursley, S.K.; Rauschel, F.M.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-06-05
Resolution : 2.40 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

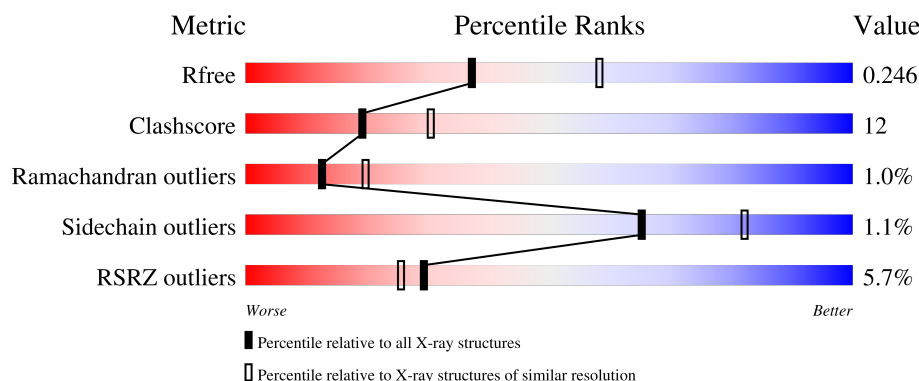
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	427	7% 69% 25% • •
1	B	427	2% 69% 24% • •
1	C	427	7% 69% 26% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10380 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 BH0493 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3393	2164	584	625	20			
1	B	412	Total	C	N	O	S	0	0	0
			3393	2164	584	625	20			
1	C	412	Total	C	N	O	S	0	0	0
			3393	2164	584	625	20			

- 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		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Na	0	0
			1	1		

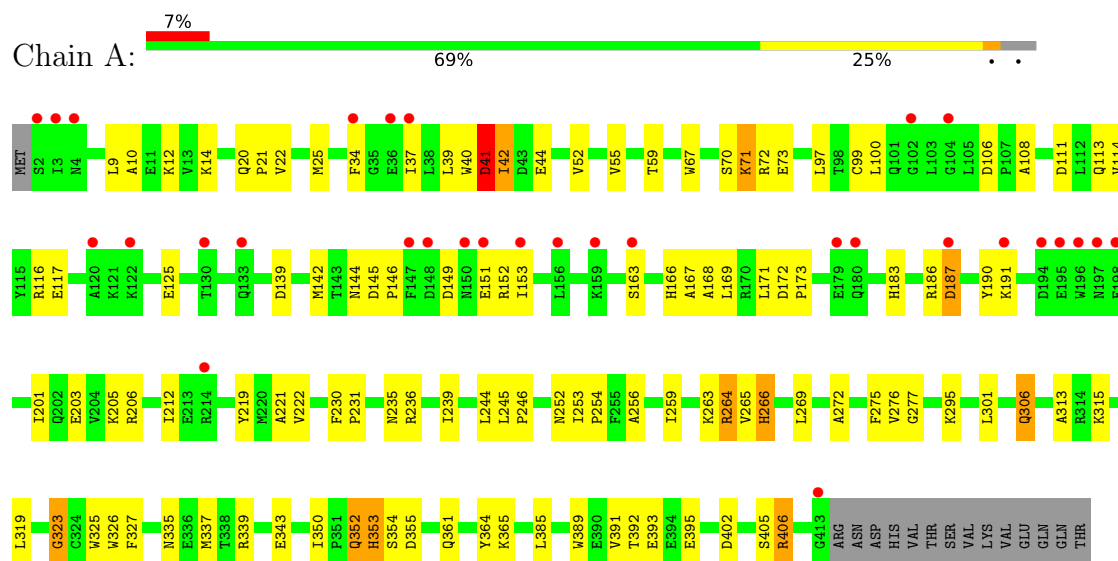
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total 53	O 53	0	0
5	B	101	Total 101	O 101	0	0
5	C	42	Total 42	O 42	0	0

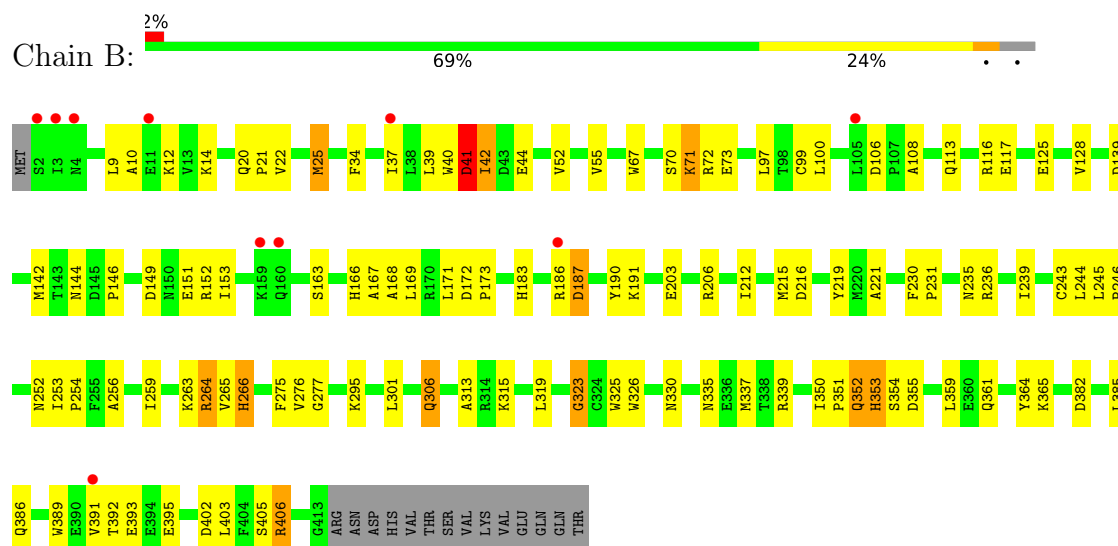
3 Residue-property plots

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: BH0493 protein

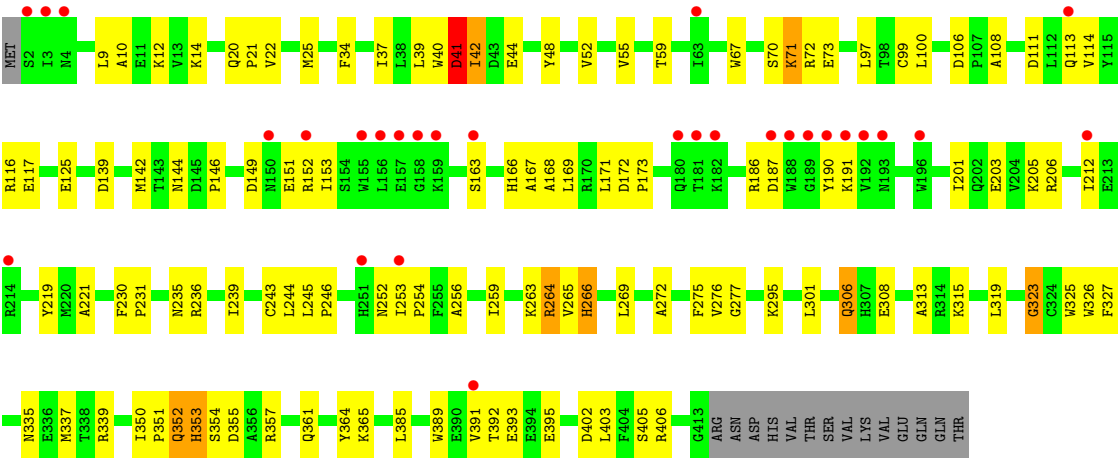


• Molecule 1: BH0493 protein



• Molecule 1: BH0493 protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.37Å 133.37Å 196.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.99 – 2.40 24.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.0 (24.99-2.40) 92.0 (24.99-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.246 0.231 , 0.246	Depositor DCC
R_{free} test set	3486 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10380	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.00% 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, CL, NA

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	0.40	0/3477	0.93	17/4712 (0.4%)
1	B	0.42	0/3477	0.94	16/4712 (0.3%)
1	C	0.39	0/3477	0.93	16/4712 (0.3%)
All	All	0.40	0/10431	0.93	49/14136 (0.3%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	TRP	N-CA-C	8.00	121.96	109.96
1	C	325	TRP	N-CA-C	7.67	121.46	109.96
1	B	325	TRP	N-CA-C	7.26	121.30	109.76
1	A	259	ILE	N-CA-C	6.69	118.67	108.71
1	C	259	ILE	N-CA-C	6.50	118.39	108.71
1	B	259	ILE	N-CA-C	6.46	118.34	108.71
1	B	264	ARG	N-CA-C	6.29	120.07	111.39
1	C	306	GLN	N-CA-C	6.20	118.55	111.11
1	A	306	GLN	N-CA-C	6.18	118.52	111.11
1	A	264	ARG	N-CA-C	6.17	119.76	111.24
1	C	264	ARG	N-CA-C	6.10	119.81	111.39
1	A	352	GLN	N-CA-C	5.99	118.17	109.07
1	B	352	GLN	N-CA-C	5.95	118.11	109.07
1	C	352	GLN	N-CA-C	5.95	118.11	109.07
1	A	212	ILE	N-CA-C	-5.90	104.76	110.72
1	B	22	VAL	N-CA-C	5.84	117.75	108.87
1	C	263	LYS	N-CA-C	5.82	118.67	110.23
1	B	306	GLN	N-CA-C	5.82	118.11	111.02
1	C	212	ILE	N-CA-C	-5.77	104.89	110.72
1	B	350	ILE	CA-C-N	5.76	125.23	119.24
1	B	350	ILE	C-N-CA	5.76	125.23	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	ILE	N-CA-C	-5.72	104.94	110.72
1	A	22	VAL	N-CA-C	5.69	117.53	108.87
1	C	350	ILE	CA-C-N	5.68	125.15	119.24
1	C	350	ILE	C-N-CA	5.68	125.15	119.24
1	B	353	HIS	N-CA-C	-5.60	100.56	109.07
1	A	350	ILE	CA-C-N	5.57	125.03	119.24
1	A	350	ILE	C-N-CA	5.57	125.03	119.24
1	B	406	ARG	N-CA-C	5.54	117.31	111.28
1	C	22	VAL	N-CA-C	5.53	117.27	108.87
1	A	263	LYS	N-CA-C	5.50	118.21	110.23
1	C	25	MET	N-CA-C	5.49	120.95	113.37
1	B	263	LYS	N-CA-C	5.46	118.37	110.28
1	A	59	THR	N-CA-C	5.46	117.78	110.35
1	B	25	MET	N-CA-C	5.42	120.85	113.37
1	B	42	ILE	N-CA-C	-5.37	104.38	111.09
1	C	353	HIS	N-CA-C	-5.32	100.98	109.07
1	C	42	ILE	N-CA-C	-5.28	104.49	111.09
1	A	353	HIS	N-CA-C	-5.28	101.05	109.07
1	A	25	MET	N-CA-C	5.22	120.57	113.37
1	A	406	ARG	N-CA-C	5.18	116.92	111.28
1	A	266	HIS	CA-C-N	5.08	124.53	119.24
1	A	266	HIS	C-N-CA	5.08	124.53	119.24
1	C	59	THR	N-CA-C	5.08	117.26	110.35
1	B	266	HIS	CA-C-N	5.06	124.50	119.24
1	B	266	HIS	C-N-CA	5.06	124.50	119.24
1	A	42	ILE	N-CA-C	-5.04	104.78	111.09
1	C	266	HIS	CA-C-N	5.03	124.47	119.24
1	C	266	HIS	C-N-CA	5.03	124.47	119.24

There are no chirality outliers.

There are no planarity outliers.

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	3393	0	3315	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3393	0	3315	81	0
1	C	3393	0	3315	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	53	0	0	2	0
5	B	101	0	0	3	0
5	C	42	0	0	3	0
All	All	10380	0	9945	236	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 12.

All (236) 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:335:ASN:HD21	1:C:339:ARG:HE	1.09	0.97
1:A:335:ASN:HD21	1:A:339:ARG:HE	1.06	0.96
1:B:335:ASN:HD21	1:B:339:ARG:HE	1.06	0.94
1:B:72:ARG:HB2	1:B:72:ARG:HH11	1.37	0.90
1:A:72:ARG:HB2	1:A:72:ARG:HH11	1.37	0.89
1:C:72:ARG:HB2	1:C:72:ARG:HH11	1.36	0.89
1:B:34:PHE:HB3	1:B:37:ILE:HD11	1.65	0.79
1:A:34:PHE:HB3	1:A:37:ILE:HD11	1.66	0.78
1:A:335:ASN:ND2	1:A:339:ARG:HE	1.83	0.77
1:C:34:PHE:HB3	1:C:37:ILE:HD11	1.66	0.76
1:C:335:ASN:ND2	1:C:339:ARG:HE	1.84	0.76
1:A:315:LYS:O	1:B:266:HIS:HD2	1.68	0.75
1:B:335:ASN:ND2	1:B:339:ARG:HE	1.83	0.75
1:C:236:ARG:HD2	5:C:507:HOH:O	1.88	0.74
1:A:72:ARG:HB2	1:A:72:ARG:NH1	2.03	0.73
1:C:72:ARG:HB2	1:C:72:ARG:NH1	2.03	0.73
1:B:72:ARG:HB2	1:B:72:ARG:NH1	2.04	0.72
1:A:266:HIS:HD2	1:C:315:LYS:O	1.77	0.68
1:A:144:ASN:HD22	1:A:168:ALA:H	1.44	0.66
1:A:144:ASN:HA	1:A:151:GLU:OE2	1.95	0.66
1:B:323:GLY:HA2	1:B:352:GLN:HA	1.78	0.65
1:A:323:GLY:HA2	1:A:352:GLN:HA	1.79	0.65
1:B:144:ASN:HD22	1:B:168:ALA:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ASN:HA	1:C:151:GLU:OE2	1.96	0.64
1:B:144:ASN:HA	1:B:151:GLU:OE2	1.97	0.64
1:B:41:ASP:HB2	1:B:44:GLU:HG2	1.80	0.64
1:B:402:ASP:HA	1:B:406:ARG:HB2	1.79	0.63
1:B:354:SER:HB2	1:B:365:LYS:HG2	1.81	0.63
1:C:41:ASP:HB2	1:C:44:GLU:HG2	1.80	0.63
1:C:323:GLY:HA2	1:C:352:GLN:HA	1.79	0.62
1:A:354:SER:HB2	1:A:365:LYS:HG2	1.80	0.62
1:C:144:ASN:HD22	1:C:168:ALA:H	1.46	0.62
1:A:236:ARG:HD2	5:A:517:HOH:O	1.99	0.62
1:C:354:SER:HB2	1:C:365:LYS:HG2	1.82	0.62
1:C:402:ASP:HA	1:C:406:ARG:HB2	1.82	0.61
1:B:315:LYS:O	1:C:266:HIS:HD2	1.83	0.61
1:A:41:ASP:HB2	1:A:44:GLU:HG2	1.80	0.61
1:C:252:ASN:ND2	1:C:295:LYS:HE2	2.16	0.60
1:A:402:ASP:HA	1:A:406:ARG:HB2	1.83	0.60
1:A:252:ASN:ND2	1:A:295:LYS:HE2	2.18	0.59
1:B:25:MET:HG3	5:B:515:HOH:O	2.02	0.58
1:B:40:TRP:O	1:B:41:ASP:HB2	2.03	0.58
1:B:252:ASN:ND2	1:B:295:LYS:HE2	2.18	0.58
1:B:392:THR:OG1	1:B:395:GLU:HG3	2.04	0.57
1:C:392:THR:OG1	1:C:395:GLU:HG3	2.05	0.57
1:A:40:TRP:O	1:A:41:ASP:HB2	2.04	0.57
1:C:40:TRP:O	1:C:41:ASP:HB2	2.03	0.57
1:C:144:ASN:ND2	1:C:167:ALA:HA	2.19	0.56
1:A:42:ILE:HD13	1:A:100:LEU:HD21	1.88	0.56
1:A:144:ASN:ND2	1:A:167:ALA:HA	2.21	0.56
1:B:144:ASN:ND2	1:B:167:ALA:HA	2.21	0.55
1:B:42:ILE:HD13	1:B:100:LEU:HD21	1.88	0.55
1:A:392:THR:OG1	1:A:395:GLU:HG3	2.06	0.55
1:B:70:SER:OG	1:B:73:GLU:HG3	2.06	0.55
1:B:306:GLN:OE1	1:B:337:MET:HE3	2.06	0.55
1:B:40:TRP:O	1:B:41:ASP:CB	2.55	0.54
1:C:42:ILE:HD13	1:C:100:LEU:HD21	1.90	0.54
1:B:236:ARG:HD2	5:B:511:HOH:O	2.08	0.54
1:A:70:SER:OG	1:A:73:GLU:HG3	2.07	0.54
1:A:301:LEU:HD11	1:A:326:TRP:HB3	1.88	0.54
1:C:149:ASP:O	1:C:153:ILE:HG13	2.08	0.54
1:C:301:LEU:HD11	1:C:326:TRP:HB3	1.89	0.53
1:B:301:LEU:CD1	1:B:326:TRP:HB3	2.39	0.53
1:B:149:ASP:O	1:B:153:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:TRP:O	1:C:41:ASP:CB	2.56	0.53
1:B:313:ALA:HA	1:B:319:LEU:HD23	1.91	0.53
1:A:306:GLN:OE1	1:A:337:MET:HE3	2.09	0.53
1:A:40:TRP:O	1:A:41:ASP:CB	2.56	0.53
1:A:149:ASP:O	1:A:153:ILE:HG13	2.10	0.52
1:A:301:LEU:CD1	1:A:326:TRP:HB3	2.38	0.52
1:A:144:ASN:HD21	1:A:167:ALA:HA	1.75	0.52
1:B:301:LEU:HD11	1:B:326:TRP:HB3	1.90	0.52
1:A:172:ASP:HB2	1:A:173:PRO:HD3	1.92	0.52
1:A:219:TYR:HA	1:A:253:ILE:CG2	2.39	0.52
1:C:301:LEU:CD1	1:C:326:TRP:HB3	2.40	0.51
1:C:144:ASN:HD21	1:C:167:ALA:HA	1.73	0.51
1:C:252:ASN:HD21	1:C:295:LYS:HE2	1.74	0.51
1:C:313:ALA:HA	1:C:319:LEU:HD23	1.93	0.51
1:C:70:SER:OG	1:C:73:GLU:HG3	2.09	0.51
1:C:219:TYR:HA	1:C:253:ILE:CG2	2.39	0.51
1:B:186:ARG:HA	1:B:190:TYR:O	2.11	0.51
1:C:172:ASP:HB2	1:C:173:PRO:HD3	1.93	0.50
1:C:44:GLU:OE1	1:C:44:GLU:HA	2.12	0.50
1:A:252:ASN:HD21	1:A:295:LYS:HE2	1.76	0.50
1:C:186:ARG:HA	1:C:190:TYR:O	2.12	0.50
1:B:252:ASN:HD21	1:B:295:LYS:HE2	1.75	0.50
1:C:306:GLN:OE1	1:C:337:MET:HE3	2.11	0.50
1:C:308:GLU:HG2	5:C:514:HOH:O	2.11	0.50
1:B:44:GLU:OE1	1:B:71:LYS:HD3	2.11	0.50
1:B:219:TYR:HA	1:B:253:ILE:CG2	2.41	0.49
1:A:276:VAL:HG22	1:A:277:GLY:N	2.28	0.49
1:B:144:ASN:HD21	1:B:167:ALA:HA	1.76	0.49
1:C:361:GLN:O	1:C:365:LYS:HB2	2.12	0.49
1:A:389:TRP:HB2	1:B:97:LEU:HD13	1.95	0.49
1:A:44:GLU:HA	1:A:44:GLU:OE1	2.12	0.49
1:C:44:GLU:OE1	1:C:71:LYS:HD3	2.13	0.49
1:B:39:LEU:HD22	1:B:44:GLU:OE2	2.13	0.48
1:B:265:VAL:HG21	1:B:275:PHE:HB2	1.96	0.48
1:C:265:VAL:HG21	1:C:275:PHE:HB2	1.94	0.48
1:B:44:GLU:OE1	1:B:44:GLU:HA	2.13	0.48
1:A:146:PRO:O	1:A:152:ARG:HD3	2.14	0.48
1:A:186:ARG:HA	1:A:190:TYR:O	2.14	0.48
1:A:169:LEU:HG	1:A:171:LEU:HD21	1.96	0.48
1:B:10:ALA:O	1:B:14:LYS:HG3	2.13	0.48
1:C:41:ASP:HB2	1:C:44:GLU:CG	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LYS:HD2	1:A:393:GLU:OE1	2.14	0.48
1:A:313:ALA:HA	1:A:319:LEU:HD23	1.96	0.48
1:B:361:GLN:O	1:B:365:LYS:HB2	2.13	0.48
1:C:39:LEU:HD22	1:C:44:GLU:OE2	2.13	0.48
1:A:335:ASN:HD21	1:A:339:ARG:NE	1.91	0.48
1:C:146:PRO:O	1:C:152:ARG:HD3	2.14	0.48
1:A:44:GLU:OE1	1:A:71:LYS:HD3	2.14	0.47
1:A:142:MET:HE3	1:A:144:ASN:HD21	1.79	0.47
1:B:385:LEU:CD1	1:B:391:VAL:HG12	2.44	0.47
1:C:276:VAL:HG22	1:C:277:GLY:N	2.28	0.47
1:A:41:ASP:HB2	1:A:44:GLU:CG	2.43	0.47
1:C:142:MET:HE3	1:C:144:ASN:HD21	1.80	0.47
1:A:39:LEU:HD22	1:A:44:GLU:OE2	2.14	0.47
1:A:42:ILE:HG22	5:A:548:HOH:O	2.14	0.47
1:A:106:ASP:OD2	1:A:108:ALA:HB3	2.13	0.47
1:B:221:ALA:HB2	1:B:256:ALA:HB3	1.97	0.47
1:C:235:ASN:O	1:C:239:ILE:HG13	2.14	0.47
1:A:385:LEU:CD1	1:A:391:VAL:HG12	2.44	0.47
1:B:172:ASP:HB2	1:B:173:PRO:HD3	1.96	0.47
1:B:191:LYS:N	1:B:191:LYS:HD2	2.30	0.47
1:B:41:ASP:HB2	1:B:44:GLU:CG	2.44	0.47
1:B:146:PRO:O	1:B:152:ARG:HD3	2.15	0.47
1:B:389:TRP:HB2	1:C:97:LEU:HD13	1.96	0.47
1:A:244:LEU:HD13	1:A:244:LEU:C	2.40	0.47
1:C:221:ALA:HB2	1:C:256:ALA:HB3	1.97	0.47
1:A:125:GLU:CD	1:A:125:GLU:H	2.23	0.46
1:A:221:ALA:HB2	1:A:256:ALA:HB3	1.97	0.46
1:C:99:CYS:HG	1:C:364:TYR:HD2	1.64	0.46
1:C:385:LEU:CD1	1:C:391:VAL:HG12	2.45	0.46
1:B:12:LYS:HD2	1:B:393:GLU:OE1	2.15	0.46
1:B:106:ASP:OD2	1:B:108:ALA:HB3	2.15	0.46
1:C:152:ARG:HH11	1:C:152:ARG:HB2	1.79	0.46
1:A:10:ALA:O	1:A:14:LYS:HG3	2.15	0.46
1:A:97:LEU:HD13	1:C:389:TRP:HB2	1.98	0.46
1:C:10:ALA:O	1:C:14:LYS:HG3	2.16	0.46
1:A:264:ARG:NH1	1:A:264:ARG:HB2	2.31	0.46
1:C:125:GLU:CD	1:C:125:GLU:H	2.23	0.46
1:A:265:VAL:HG21	1:A:275:PHE:HB2	1.98	0.46
1:C:20:GLN:NE2	1:C:21:PRO:HD2	2.31	0.45
1:A:113:GLN:HE22	1:A:116:ARG:NH1	2.14	0.45
1:A:352:GLN:HG3	1:A:353:HIS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:OD2	1:C:108:ALA:HB3	2.16	0.45
1:A:20:GLN:NE2	1:A:21:PRO:HD2	2.31	0.45
1:B:67:TRP:CE3	1:B:67:TRP:HA	2.51	0.45
1:B:113:GLN:O	1:B:117:GLU:HG3	2.16	0.45
1:B:113:GLN:HE22	1:B:116:ARG:NH1	2.15	0.45
1:B:191:LYS:HE3	1:B:191:LYS:HA	1.98	0.45
1:A:67:TRP:HA	1:A:67:TRP:CE3	2.51	0.45
1:B:276:VAL:HG22	1:B:277:GLY:N	2.32	0.45
1:C:12:LYS:HD2	1:C:393:GLU:OE1	2.16	0.45
1:A:152:ARG:HH11	1:A:152:ARG:HB2	1.82	0.45
1:B:151:GLU:HG2	5:B:583:HOH:O	2.16	0.45
1:C:244:LEU:HD13	1:C:244:LEU:C	2.42	0.45
1:A:52:VAL:O	1:A:55:VAL:HG12	2.17	0.45
1:C:52:VAL:O	1:C:55:VAL:HG12	2.17	0.44
1:C:113:GLN:HE22	1:C:116:ARG:NH1	2.14	0.44
1:B:254:PRO:HG3	1:B:295:LYS:HE3	2.00	0.44
1:C:191:LYS:HE3	1:C:191:LYS:HA	2.00	0.44
1:A:254:PRO:HG3	1:A:295:LYS:HE3	1.98	0.44
1:B:142:MET:HE3	1:B:144:ASN:HD21	1.82	0.44
1:B:203:GLU:OE1	1:B:206:ARG:NH1	2.50	0.44
1:B:235:ASN:O	1:B:239:ILE:HG13	2.17	0.44
1:C:9:LEU:HD22	1:C:385:LEU:HD22	2.00	0.44
1:C:67:TRP:HA	1:C:67:TRP:CE3	2.52	0.44
1:A:191:LYS:HE3	1:A:191:LYS:HA	2.00	0.44
1:A:99:CYS:HG	1:A:364:TYR:HD2	1.66	0.44
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.44
1:B:244:LEU:C	1:B:244:LEU:HD13	2.43	0.44
1:B:352:GLN:HG3	1:B:353:HIS:N	2.32	0.44
1:C:169:LEU:HG	1:C:171:LEU:HD21	2.00	0.44
1:C:243:CYS:C	1:C:246:PRO:HD2	2.43	0.44
1:A:361:GLN:O	1:A:365:LYS:HB2	2.17	0.44
1:C:264:ARG:HB2	1:C:264:ARG:NH1	2.33	0.44
1:C:191:LYS:HD2	1:C:191:LYS:N	2.33	0.43
1:C:352:GLN:HG3	1:C:353:HIS:N	2.32	0.43
1:A:113:GLN:O	1:A:117:GLU:HG3	2.17	0.43
1:A:203:GLU:OE1	1:A:206:ARG:NH1	2.51	0.43
1:B:152:ARG:HB2	1:B:152:ARG:HH11	1.83	0.43
1:C:236:ARG:NH2	5:C:543:HOH:O	2.51	0.43
1:B:20:GLN:NE2	1:B:21:PRO:HD2	2.33	0.43
1:B:139:ASP:OD1	1:B:166:HIS:HE1	2.01	0.43
1:A:72:ARG:HG3	1:A:116:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD1	1:A:166:HIS:HE1	2.01	0.43
1:B:52:VAL:O	1:B:55:VAL:HG12	2.19	0.43
1:B:335:ASN:HD21	1:B:339:ARG:NE	1.91	0.43
1:B:9:LEU:HD22	1:B:385:LEU:HD22	2.01	0.43
1:C:351:PRO:HG2	1:C:403:LEU:HB3	2.01	0.43
1:A:275:PHE:CG	1:A:276:VAL:N	2.87	0.43
1:C:139:ASP:OD1	1:C:166:HIS:HE1	2.02	0.43
1:C:201:ILE:O	1:C:205:LYS:HG3	2.19	0.43
1:A:245:LEU:HB2	1:A:246:PRO:HD3	2.01	0.42
1:B:382:ASP:O	1:B:386:GLN:HG2	2.19	0.42
1:A:111:ASP:CG	1:A:114:VAL:HG23	2.44	0.42
1:B:169:LEU:HG	1:B:171:LEU:HD21	2.01	0.42
1:B:243:CYS:C	1:B:246:PRO:HD2	2.44	0.42
1:C:113:GLN:O	1:C:117:GLU:HG3	2.18	0.42
1:B:125:GLU:CD	1:B:125:GLU:H	2.27	0.42
1:B:264:ARG:NH1	1:B:264:ARG:HB2	2.33	0.42
1:C:111:ASP:CG	1:C:114:VAL:HG23	2.44	0.42
1:A:235:ASN:O	1:A:239:ILE:HG13	2.20	0.42
1:A:9:LEU:HD22	1:A:385:LEU:HD22	2.01	0.42
1:A:230:PHE:HA	1:A:231:PRO:C	2.45	0.42
1:A:326:TRP:HB3	1:A:327:PHE:H	1.65	0.42
1:C:254:PRO:HG3	1:C:295:LYS:HE3	2.00	0.42
1:A:269:LEU:HB3	1:A:272:ALA:HB3	2.02	0.42
1:B:230:PHE:HA	1:B:231:PRO:C	2.45	0.42
1:B:99:CYS:HG	1:B:364:TYR:HD2	1.67	0.42
1:A:183:HIS:O	1:A:187:ASP:HB2	2.20	0.42
1:C:230:PHE:HA	1:C:231:PRO:C	2.44	0.42
1:A:201:ILE:O	1:A:205:LYS:HG3	2.19	0.42
1:C:203:GLU:OE1	1:C:206:ARG:NH1	2.53	0.42
1:A:12:LYS:HD2	1:A:393:GLU:CD	2.45	0.41
1:C:113:GLN:HE22	1:C:116:ARG:HH11	1.69	0.41
1:C:48:TYR:HE1	1:C:357:ARG:HD2	1.86	0.41
1:C:245:LEU:HB2	1:C:246:PRO:HD3	2.02	0.41
1:A:172:ASP:OD1	1:A:222:VAL:HA	2.21	0.41
1:B:12:LYS:HD2	1:B:393:GLU:CD	2.46	0.41
1:A:145:ASP:HA	1:A:146:PRO:HD2	1.96	0.41
1:C:326:TRP:HB3	1:C:327:PHE:H	1.66	0.41
1:B:183:HIS:O	1:B:187:ASP:HB2	2.21	0.41
1:B:351:PRO:HG2	1:B:403:LEU:HB3	2.02	0.41
1:C:12:LYS:HD2	1:C:393:GLU:CD	2.46	0.41
1:B:20:GLN:HA	1:B:21:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:HB2	1:B:246:PRO:HD3	2.01	0.41
1:C:142:MET:O	1:C:168:ALA:HB3	2.21	0.41
1:C:269:LEU:HB3	1:C:272:ALA:HB3	2.03	0.41
1:A:343:GLU:OE1	1:B:330:ASN:HB3	2.21	0.40
1:B:128:VAL:HA	1:B:359:LEU:HD21	2.03	0.40
1:B:215:MET:O	1:B:216:ASP:C	2.64	0.40
1:B:72:ARG:HG3	1:B:116:ARG:NH2	2.36	0.40
1:C:20:GLN:HA	1:C:21:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

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	410/427 (96%)	394 (96%)	12 (3%)	4 (1%)	12	20
1	B	410/427 (96%)	395 (96%)	11 (3%)	4 (1%)	12	20
1	C	410/427 (96%)	394 (96%)	12 (3%)	4 (1%)	12	20
All	All	1230/1281 (96%)	1183 (96%)	35 (3%)	12 (1%)	12	20

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	B	41	ASP
1	C	41	ASP
1	A	323	GLY
1	A	163	SER
1	B	163	SER
1	C	163	SER
1	A	405	SER
1	C	405	SER

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Mol	Chain	Res	Type
1	B	405	SER
1	C	323	GLY
1	B	323	GLY

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	372/387 (96%)	368 (99%)	4 (1%)	65	82
1	B	372/387 (96%)	368 (99%)	4 (1%)	65	82
1	C	372/387 (96%)	368 (99%)	4 (1%)	65	82
All	All	1116/1161 (96%)	1104 (99%)	12 (1%)	65	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ASP
1	A	71	LYS
1	A	187	ASP
1	A	355	ASP
1	B	41	ASP
1	B	71	LYS
1	B	187	ASP
1	B	355	ASP
1	C	41	ASP
1	C	71	LYS
1	C	187	ASP
1	C	355	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	49	HIS
1	A	113	GLN
1	A	133	GLN
1	A	144	ASN
1	A	166	HIS
1	A	183	HIS
1	A	235	ASN
1	A	252	ASN
1	A	266	HIS
1	A	294	ASN
1	A	335	ASN
1	B	15	ASN
1	B	20	GLN
1	B	49	HIS
1	B	113	GLN
1	B	133	GLN
1	B	144	ASN
1	B	166	HIS
1	B	183	HIS
1	B	235	ASN
1	B	252	ASN
1	B	266	HIS
1	B	294	ASN
1	B	335	ASN
1	C	15	ASN
1	C	20	GLN
1	C	49	HIS
1	C	113	GLN
1	C	133	GLN
1	C	144	ASN
1	C	166	HIS
1	C	183	HIS
1	C	235	ASN
1	C	252	ASN
1	C	266	HIS
1	C	294	ASN
1	C	335	ASN

5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 5 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	412/427 (96%)	0.45	31 (7%)	20 17	22, 44, 65, 76	0
1	B	412/427 (96%)	0.03	10 (2%)	59 55	18, 35, 56, 71	0
1	C	412/427 (96%)	0.54	29 (7%)	22 19	24, 49, 70, 80	0
All	All	1236/1281 (96%)	0.34	70 (5%)	29 25	18, 43, 66, 80	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	GLN	5.7
1	A	150	ASN	5.2
1	A	2	SER	4.3
1	A	194	ASP	4.1
1	C	2	SER	4.1
1	C	193	ASN	3.6
1	A	195	GLU	3.5
1	B	2	SER	3.4
1	B	4	ASN	3.3
1	C	3	ILE	3.3
1	A	151	GLU	3.3
1	C	158	GLY	3.0
1	A	153	ILE	3.0
1	C	159	LYS	3.0
1	A	198	GLU	3.0
1	A	148	ASP	3.0
1	A	37	ILE	2.9
1	A	147	PHE	2.9
1	C	163	SER	2.9
1	C	189	GLY	2.9
1	B	3	ILE	2.8
1	A	191	LYS	2.8
1	A	3	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	190	TYR	2.8
1	B	37	ILE	2.7
1	A	4	ASN	2.7
1	C	191	LYS	2.7
1	C	187	ASP	2.7
1	A	104	GLY	2.6
1	A	159	LYS	2.6
1	C	152	ARG	2.6
1	C	157	GLU	2.5
1	B	159	LYS	2.5
1	A	196	TRP	2.5
1	A	156	LEU	2.5
1	C	63	ILE	2.4
1	C	214	ARG	2.4
1	C	251	HIS	2.4
1	A	163	SER	2.3
1	A	180	GLN	2.3
1	A	34	PHE	2.3
1	C	181	THR	2.3
1	C	196	TRP	2.3
1	A	413	GLY	2.3
1	A	102	GLY	2.2
1	C	180	GLN	2.2
1	C	188	TRP	2.2
1	A	214	ARG	2.2
1	B	105	LEU	2.2
1	C	156	LEU	2.2
1	A	179	GLU	2.2
1	C	150	ASN	2.2
1	C	4	ASN	2.1
1	C	155	TRP	2.1
1	A	120	ALA	2.1
1	C	253	ILE	2.1
1	B	11	GLU	2.1
1	A	36	GLU	2.1
1	C	113	GLN	2.1
1	B	186	ARG	2.1
1	A	130	THR	2.1
1	A	122	LYS	2.1
1	A	187	ASP	2.1
1	B	160	GLN	2.0
1	B	391	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	192	VAL	2.0
1	C	182	LYS	2.0
1	C	212	ILE	2.0
1	C	391	VAL	2.0
1	A	197	ASN	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	501	1/1	0.98	0.03	45,45,45,45	0
2	ZN	C	503	1/1	0.98	0.04	60,60,60,60	0
4	NA	C	504	1/1	0.98	0.09	33,33,33,33	0
3	CL	A	502	1/1	0.99	0.04	24,24,24,24	0
2	ZN	B	502	1/1	0.99	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.