



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:39 PM GMT

PDB ID : 3HM7
Title : Crystal structure of allantoinase from *Bacillus halodurans* C-125
Authors : Patskovsky, Y.; Romero, R.; Rutter, M.; Miller, S.; Wasserman, S.R.; Sauder, J.M.; Raushel, F.M.; Burley, S.K.; Almo, S.C.; New York Structural Genomix Research Consortium (Nysgxrc); New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-05-28
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

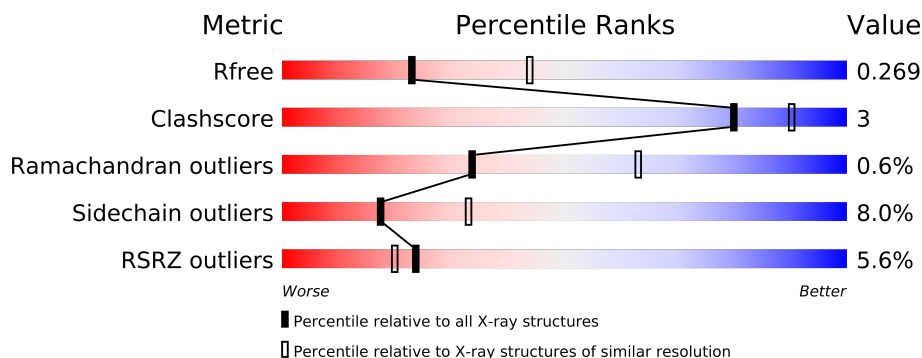
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	
1	F	448	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZN	E	447	-	X
2	ZN	F	447	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20901 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Allantoinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	4	0
			3425	2166	593	649	17			
1	B	437	Total	C	N	O	S	0	5	0
			3437	2173	594	653	17			
1	C	435	Total	C	N	O	S	0	3	0
			3410	2154	588	651	17			
1	D	436	Total	C	N	O	S	0	2	0
			3415	2157	591	650	17			
1	E	436	Total	C	N	O	S	0	2	0
			3412	2156	590	649	17			
1	F	436	Total	C	N	O	S	0	4	0
			3425	2165	592	651	17			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
A	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
A	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
A	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
A	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
A	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
A	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
B	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
B	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
B	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
B	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
B	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
B	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
C	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
C	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
C	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
C	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
C	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
C	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
D	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
D	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
D	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
D	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
D	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
D	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
E	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
E	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
E	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8
E	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
E	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
E	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	-1	MET	-	EXPRESSION TAG	UNP Q9KAH8
F	0	SER	-	EXPRESSION TAG	UNP Q9KAH8
F	1	LEU	-	EXPRESSION TAG	UNP Q9KAH8
F	439	GLU	-	EXPRESSION TAG	UNP Q9KAH8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	GLY	-	EXPRESSION TAG	UNP Q9KAH8
F	441	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	442	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	443	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	444	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	445	HIS	-	EXPRESSION TAG	UNP Q9KAH8
F	446	HIS	-	EXPRESSION TAG	UNP Q9KAH8

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

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

- Molecule 3 is water.

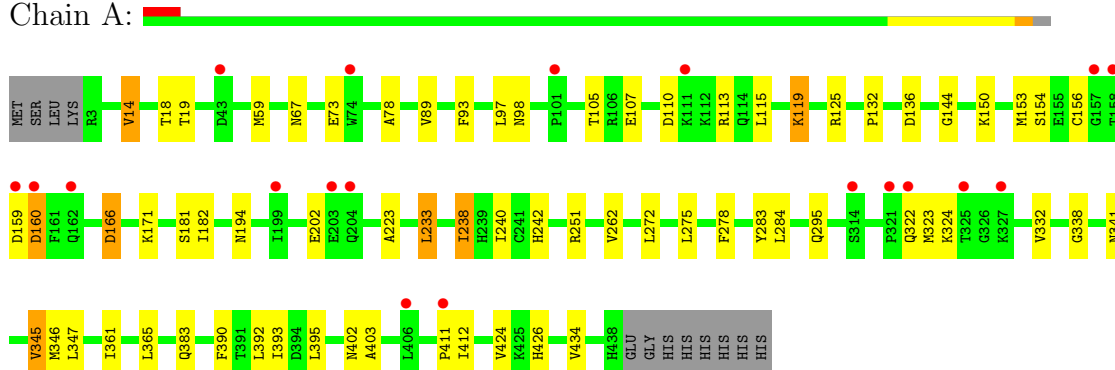
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	53	Total O 53 53	0	0
3	B	69	Total O 69 69	0	0
3	C	39	Total O 39 39	0	0
3	D	47	Total O 47 47	0	0
3	E	74	Total O 74 74	0	0
3	F	89	Total O 89 89	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

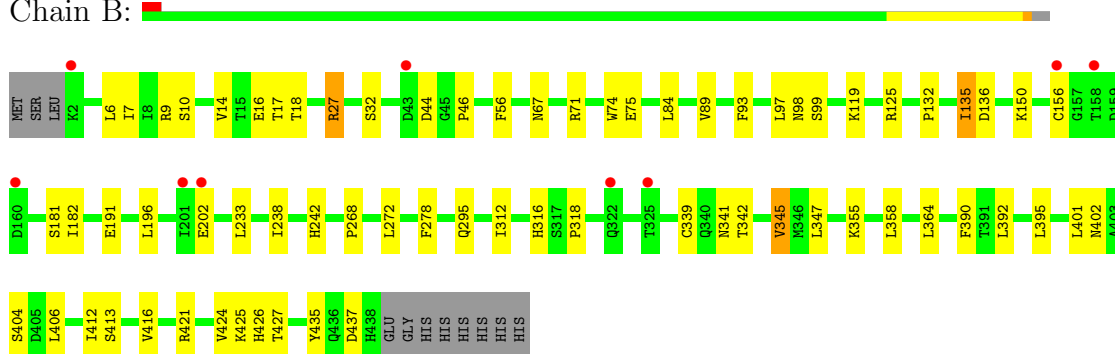
• Molecule 1: Allantoinase

Chain A:



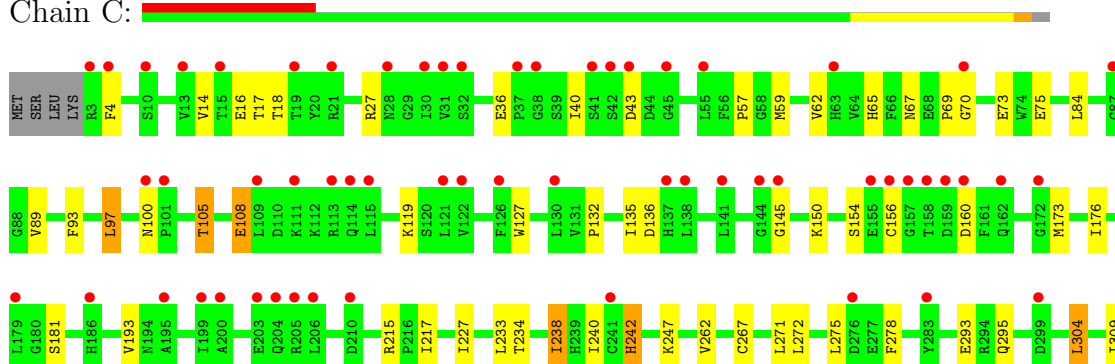
• Molecule 1: Allantoinase

Chain B:



• Molecule 1: Allantoinase

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.66Å 157.66Å 418.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60 27.39 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.60) 100.0 (27.39-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.94 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.240 , 0.267 0.244 , 0.269	Depositor DCC
R_{free} test set	2853 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	37 of 94701 reflections (0.039%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20901	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 69.84 % 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 3.4571e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.41	0/3507	0.60	0/4749
1	B	0.44	0/3523	0.61	1/4770 (0.0%)
1	C	0.43	0/3485	0.62	0/4720
1	D	0.42	0/3488	0.59	0/4724
1	E	0.43	0/3488	0.59	0/4724
1	F	0.41	0/3508	0.61	1/4752 (0.0%)
All	All	0.42	0/20999	0.60	2/28439 (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	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	LEU	CA-CB-CG	6.19	129.54	115.30
1	F	262	VAL	CB-CA-C	-5.13	101.65	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ASP	Peptide
1	A	160	ASP	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3425	0	3404	27	0
1	B	3437	0	3411	25	0
1	C	3410	0	3376	32	0
1	D	3415	0	3379	29	0
1	E	3412	0	3380	16	0
1	F	3425	0	3393	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	53	0	0	0	0
3	B	69	0	0	0	0
3	C	39	0	0	0	0
3	D	47	0	0	0	0
3	E	74	0	0	0	0
3	F	89	0	0	0	0
All	All	20901	0	20343	138	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (138) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:67:ASN:ND2	1:D:98:ASN:HB2	1.96	0.80
1:F:75:GLU:HG2	1:F:318:PRO:HG3	1.69	0.73
1:B:75:GLU:HG2	1:B:318:PRO:HG3	1.76	0.68
1:F:67:ASN:ND2	1:F:98:ASN:HB2	2.09	0.67
1:E:67:ASN:ND2	1:E:98:ASN:HB2	2.09	0.67
1:B:67:ASN:ND2	1:B:98:ASN:HB2	2.10	0.67
1:D:96:PRO:HD3	1:D:127:TRP:HB2	1.76	0.67
1:D:97:LEU:O	1:D:98:ASN:HB2	1.94	0.66
1:A:393:ILE:HG22	1:A:395:LEU:HD23	1.78	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:283:TYR:HE1	1:D:329:ILE:HA	1.63	0.62
1:C:70:GLY:HA3	1:C:100:ASN:H	1.64	0.62
1:F:16[B]:GLU:HG3	1:F:17:THR:HG23	1.83	0.61
1:C:359:THR:HG22	1:C:360:GLN:N	2.16	0.60
1:A:18:THR:HG21	1:E:383:GLN:HE22	1.67	0.60
1:B:18:THR:HG21	1:F:383:GLN:HE22	1.67	0.60
1:D:67:ASN:ND2	1:D:98:ASN:CB	2.64	0.59
1:B:316:HIS:HB2	1:B:339:CYS:HB3	1.85	0.58
1:A:14:VAL:HG12	1:A:19:THR:HG22	1.86	0.58
1:E:16[B]:GLU:HG3	1:E:17:THR:HG23	1.86	0.57
1:C:359:THR:CG2	1:C:360:GLN:N	2.67	0.57
1:E:65:HIS:HB3	1:E:67:ASN:HD21	1.69	0.57
1:C:18:THR:HG21	1:D:383:GLN:HE22	1.68	0.57
1:D:346:MET:HG3	1:D:365:LEU:HD11	1.88	0.55
1:D:283:TYR:CE1	1:D:329:ILE:HA	2.40	0.55
1:B:84:LEU:HB3	1:B:89:VAL:HB	1.87	0.55
1:B:9:ARG:O	1:B:10:SER:HB2	2.07	0.55
1:C:62:VAL:HA	1:C:93:PHE:HB2	1.89	0.54
1:B:392:LEU:HB2	1:B:426:HIS:HB2	1.90	0.54
1:D:97:LEU:C	1:D:99:SER:H	2.12	0.53
1:F:427:THR:HB	1:F:435:TYR:HB3	1.91	0.53
1:A:18:THR:HG21	1:E:383:GLN:NE2	2.23	0.53
1:B:56:PHE:HZ	1:B:358:LEU:HD22	1.73	0.53
1:B:268:PRO:HG3	1:B:342:THR:HG23	1.91	0.53
1:C:238:ILE:HD11	1:C:240:ILE:HD11	1.91	0.53
1:F:433:HIS:HE1	1:F:436:GLN:HB2	1.73	0.52
1:D:316:HIS:HB2	1:D:339:CYS:HB3	1.91	0.52
1:C:4:PHE:HE2	1:C:40:ILE:HG12	1.75	0.52
1:D:84:LEU:HB3	1:D:89:VAL:HB	1.90	0.52
1:F:65:HIS:HB3	1:F:67:ASN:HD21	1.75	0.52
1:C:346:MET:HG3	1:C:365:LEU:HD11	1.91	0.52
1:D:50:GLY:HA2	1:D:53:LEU:HD12	1.91	0.51
1:C:368:GLU:HA	1:C:371:LYS:HB2	1.92	0.51
1:A:166:ASP:HB2	1:B:191:GLU:HG3	1.93	0.51
1:D:59:MET:HB2	1:D:89:VAL:HG22	1.93	0.51
1:A:403:ALA:HB1	1:A:411:PRO:HB2	1.93	0.51
1:D:96:PRO:HD3	1:D:127:TRP:CB	2.41	0.50
1:C:65:HIS:HB3	1:C:67:ASN:HD21	1.77	0.50
1:C:401:LEU:HD21	1:C:406:LEU:HD21	1.94	0.50
1:D:401:LEU:HD21	1:D:406:LEU:HD21	1.92	0.50
1:C:16[A]:GLU:HG2	1:C:17:THR:HG23	1.93	0.50
1:F:93:PHE:CD1	1:F:125:ARG:HB2	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:16[B]:GLU:HG3	1:D:17:THR:HG23	1.94	0.49
1:A:383:GLN:NE2	1:E:18:THR:HG21	2.28	0.49
1:A:78:ALA:HB2	1:A:119:LYS:HG3	1.95	0.48
1:A:341:ASN:O	1:A:345:VAL:HG12	2.13	0.48
1:E:346:MET:HG3	1:E:365:LEU:HD11	1.96	0.48
1:B:16[B]:GLU:HG3	1:B:17:THR:HG23	1.95	0.47
1:C:173:MET:HB3	1:C:234:THR:HG21	1.96	0.47
1:F:176:ILE:HG23	1:F:181:SER:HB3	1.97	0.47
1:C:271:LEU:HD11	1:C:304:LEU:HD13	1.97	0.47
1:C:217:ILE:HG21	1:C:247:LYS:HD2	1.96	0.47
1:A:110:ASP:HA	1:A:113:ARG:HB3	1.97	0.47
1:A:153:MET:CE	1:A:223:ALA:HB1	2.45	0.47
1:C:267:CYS:SG	1:C:315:ASP:HB2	2.54	0.47
1:E:316:HIS:HB2	1:E:339:CYS:HB3	1.97	0.46
1:C:427:THR:HB	1:C:435:TYR:HB3	1.98	0.46
1:A:233:LEU:HD21	1:B:196:LEU:HD11	1.96	0.46
1:F:316:HIS:HB2	1:F:339:CYS:HB3	1.97	0.46
1:A:383:GLN:HE22	1:E:18:THR:HG21	1.81	0.46
1:F:401:LEU:HD21	1:F:406:LEU:HD21	1.96	0.46
1:C:59:MET:HA	1:C:366:SER:HB2	1.98	0.46
1:A:93:PHE:CD1	1:A:125:ARG:HB2	2.51	0.46
1:A:181:SER:OG	1:A:182:ILE:N	2.49	0.46
1:F:169:LEU:HB3	1:F:173:MET:HE3	1.98	0.46
1:D:130:LEU:HD13	1:D:138:LEU:HD11	1.98	0.46
1:F:150:LYS:NZ	1:F:241:CYS:SG	2.89	0.45
1:E:169:LEU:HB3	1:E:173:MET:HE2	1.98	0.45
1:C:304:LEU:HD12	1:C:309:ILE:HD12	1.99	0.45
1:D:6:LEU:HD11	1:D:48:ILE:HG12	1.99	0.45
1:E:401:LEU:HD21	1:E:406:LEU:HD21	1.98	0.45
1:D:352:HIS:CD2	1:D:421:ARG:HB3	2.52	0.45
1:C:84:LEU:HB3	1:C:89:VAL:HB	1.99	0.45
1:B:135:ILE:H	1:B:135:ILE:HG13	1.56	0.45
1:A:238:ILE:HD11	1:A:240:ILE:HD11	1.99	0.45
1:B:312:ILE:HG12	1:B:364:LEU:HB3	1.99	0.44
1:A:392:LEU:HB2	1:A:426:HIS:HB2	2.00	0.44
1:B:427:THR:HB	1:B:435:TYR:HB3	2.00	0.44
1:D:84:LEU:HD22	1:D:89:VAL:HG11	1.99	0.44
1:E:284:LEU:HD23	1:E:324:LYS:HG2	2.00	0.44
1:F:84:LEU:HB3	1:F:89:VAL:HB	1.99	0.44
1:B:27:ARG:HB2	1:B:32:SER:HB2	1.99	0.44
1:E:150:LYS:NZ	1:E:241:CYS:SG	2.89	0.43
1:C:105:THR:HG23	1:C:108:GLU:HB2	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:18:THR:HG21	1:F:383:GLN:NE2	2.32	0.43
1:D:312:ILE:HG12	1:D:364:LEU:HB3	1.99	0.43
1:C:93:PHE:HB3	1:C:127:TRP:NE1	2.34	0.43
1:B:401:LEU:HD21	1:B:406:LEU:HD21	1.99	0.43
1:A:346:MET:HG3	1:A:365:LEU:HD11	1.99	0.43
1:C:14:VAL:O	1:C:57:PRO:HD3	2.19	0.43
1:C:275:LEU:HB2	1:C:293:GLU:HA	2.01	0.43
1:A:284:LEU:HD23	1:A:324:LYS:HE3	2.01	0.43
1:A:275:LEU:HA	1:A:275:LEU:HD12	1.94	0.42
1:A:283:TYR:CD1	1:A:332:VAL:HG21	2.53	0.42
1:F:35:THR:HG21	1:F:40:ILE:HD13	2.01	0.42
1:D:251:ARG:HA	1:D:251:ARG:HD2	1.85	0.42
1:D:92:TYR:CZ	1:D:124:TYR:HB3	2.54	0.42
1:E:96:PRO:HD2	1:E:97:LEU:HD23	2.02	0.42
1:E:427:THR:HB	1:E:435:TYR:HB3	2.00	0.42
1:B:413:SER:HB3	1:B:416:VAL:HG23	2.02	0.42
1:B:71:ARG:HD3	1:B:74:TRP:CZ2	2.54	0.42
1:F:6:LEU:HD11	1:F:48:ILE:HG12	2.01	0.42
1:D:93:PHE:CD1	1:D:125:ARG:HB2	2.55	0.42
1:B:425:LYS:HA	1:B:437:ASP:HB2	2.02	0.42
1:B:181:SER:OG	1:B:182:ILE:N	2.50	0.41
1:A:113:ARG:NH1	1:A:144:GLY:O	2.53	0.41
1:D:169:LEU:HB3	1:D:173:MET:HE3	2.02	0.41
1:A:59:MET:HB2	1:A:89:VAL:HG22	2.01	0.41
1:D:433:HIS:HE1	1:D:436:GLN:HG3	1.85	0.41
1:C:18:THR:HG21	1:D:383:GLN:NE2	2.35	0.41
1:F:71:ARG:HD3	1:F:74:TRP:CZ2	2.55	0.41
1:C:193:VAL:HG22	1:C:215:ARG:HA	2.01	0.41
1:C:316:HIS:HB2	1:C:339:CYS:HB3	2.01	0.41
1:B:6:LEU:HD12	1:B:46:PRO:HB2	2.01	0.41
1:A:67:ASN:ND2	1:A:98:ASN:HB3	2.35	0.41
1:C:176:ILE:HG23	1:C:181:SER:HB3	2.01	0.41
1:E:50:GLY:HA2	1:E:53:LEU:HD12	2.03	0.41
1:D:238:ILE:HG23	1:D:262:VAL:HG13	2.02	0.41
1:A:153:MET:HE2	1:A:223:ALA:HB1	2.02	0.41
1:A:251:ARG:HA	1:A:251:ARG:HD2	1.94	0.41
1:D:347:LEU:HD12	1:D:347:LEU:HA	1.86	0.41
1:C:413:SER:HB3	1:C:416:VAL:HG23	2.02	0.41
1:C:65:HIS:HE1	1:C:97:LEU:HD21	1.86	0.41
1:B:93:PHE:CD1	1:B:125:ARG:HB2	2.56	0.40
1:C:16[B]:GLU:HG3	1:C:17:THR:HG23	2.02	0.40
1:C:73:GLU:H	1:C:73:GLU:HG2	1.66	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:341:ASN:O	1:B:345:VAL:HG12	2.21	0.40
1:A:283:TYR:CE1	1:A:332:VAL:HG21	2.57	0.40
1:F:366:SER:OG	1:F:380:GLY:HA2	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	438/448 (98%)	410 (94%)	25 (6%)	3 (1%)	30	58
1	B	440/448 (98%)	425 (97%)	13 (3%)	2 (0%)	38	67
1	C	436/448 (97%)	397 (91%)	35 (8%)	4 (1%)	25	49
1	D	436/448 (97%)	416 (95%)	18 (4%)	2 (0%)	38	67
1	E	436/448 (97%)	419 (96%)	15 (3%)	2 (0%)	38	67
1	F	438/448 (98%)	424 (97%)	12 (3%)	2 (0%)	38	67
All	All	2624/2688 (98%)	2491 (95%)	118 (4%)	15 (1%)	33	63

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PRO
1	A	242	HIS
1	B	242	HIS
1	C	242	HIS
1	D	242	HIS
1	E	242	HIS
1	F	242	HIS
1	D	338	GLY
1	F	338	GLY
1	C	145	GLY
1	E	338	GLY
1	B	132	PRO

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Mol	Chain	Res	Type
1	C	132	PRO
1	A	338	GLY
1	C	69	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	375/382 (98%)	343 (92%)	32 (8%)	15	29
1	B	377/382 (99%)	351 (93%)	26 (7%)	22	42
1	C	373/382 (98%)	336 (90%)	37 (10%)	11	21
1	D	373/382 (98%)	340 (91%)	33 (9%)	14	27
1	E	373/382 (98%)	350 (94%)	23 (6%)	26	49
1	F	375/382 (98%)	347 (92%)	28 (8%)	19	36
All	All	2246/2292 (98%)	2067 (92%)	179 (8%)	17	33

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	73	GLU
1	A	97	LEU
1	A	105	THR
1	A	107	GLU
1	A	115	LEU
1	A	119	LYS
1	A	136	ASP
1	A	150	LYS
1	A	154	SER
1	A	156	CYS
1	A	160	ASP
1	A	166	ASP
1	A	171	LYS
1	A	194	ASN
1	A	202	GLU

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Mol	Chain	Res	Type
1	A	233	LEU
1	A	238	ILE
1	A	262	VAL
1	A	272	LEU
1	A	278	PHE
1	A	295	GLN
1	A	322	GLN
1	A	323	MET
1	A	345	VAL
1	A	347	LEU
1	A	361	ILE
1	A	390	PHE
1	A	402	ASN
1	A	412	ILE
1	A	424	VAL
1	A	434	VAL
1	B	7	ILE
1	B	14	VAL
1	B	27	ARG
1	B	44	ASP
1	B	97	LEU
1	B	99	SER
1	B	119	LYS
1	B	135	ILE
1	B	136	ASP
1	B	150	LYS
1	B	156	CYS
1	B	202	GLU
1	B	233	LEU
1	B	238	ILE
1	B	272	LEU
1	B	278	PHE
1	B	295	GLN
1	B	345	VAL
1	B	347	LEU
1	B	355	LYS
1	B	390	PHE
1	B	402	ASN
1	B	404	SER
1	B	412	ILE
1	B	421	ARG
1	B	424	VAL

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Mol	Chain	Res	Type
1	C	27	ARG
1	C	36	GLU
1	C	43	ASP
1	C	75	GLU
1	C	97	LEU
1	C	105	THR
1	C	108	GLU
1	C	119	LYS
1	C	135	ILE
1	C	136	ASP
1	C	150	LYS
1	C	154	SER
1	C	156	CYS
1	C	160	ASP
1	C	227	ILE
1	C	233	LEU
1	C	238	ILE
1	C	242	HIS
1	C	262	VAL
1	C	272	LEU
1	C	278	PHE
1	C	295	GLN
1	C	304	LEU
1	C	310	ASP
1	C	312	ILE
1	C	328	THR
1	C	343	LEU
1	C	355	LYS
1	C	359	THR
1	C	361	ILE
1	C	378	GLN
1	C	390	PHE
1	C	393	ILE
1	C	402	ASN
1	C	418	GLN
1	C	424	VAL
1	C	434	VAL
1	D	40	ILE
1	D	44	ASP
1	D	73	GLU
1	D	103	THR
1	D	112	LYS

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Mol	Chain	Res	Type
1	D	113	ARG
1	D	119	LYS
1	D	134	ASN
1	D	135	ILE
1	D	136	ASP
1	D	140	ASP
1	D	150	LYS
1	D	154	SER
1	D	158	THR
1	D	166	ASP
1	D	202	GLU
1	D	218	VAL
1	D	233	LEU
1	D	238	ILE
1	D	262	VAL
1	D	272	LEU
1	D	278	PHE
1	D	295	GLN
1	D	322	GLN
1	D	347	LEU
1	D	390	PHE
1	D	395	LEU
1	D	402	ASN
1	D	418	GLN
1	D	421	ARG
1	D	424	VAL
1	D	434	VAL
1	D	436	GLN
1	E	14	VAL
1	E	57	PRO
1	E	97	LEU
1	E	99	SER
1	E	105	THR
1	E	113	ARG
1	E	119	LYS
1	E	134	ASN
1	E	135	ILE
1	E	150	LYS
1	E	160	ASP
1	E	175	LYS
1	E	181	SER
1	E	219	SER

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Mol	Chain	Res	Type
1	E	242	HIS
1	E	272	LEU
1	E	275	LEU
1	E	295	GLN
1	E	322	GLN
1	E	390	PHE
1	E	402	ASN
1	E	404	SER
1	E	434	VAL
1	F	14	VAL
1	F	75	GLU
1	F	97	LEU
1	F	108	GLU
1	F	113	ARG
1	F	114	GLN
1	F	119	LYS
1	F	134	ASN
1	F	136	ASP
1	F	150	LYS
1	F	160	ASP
1	F	171	LYS
1	F	202	GLU
1	F	233	LEU
1	F	242	HIS
1	F	262	VAL
1	F	272	LEU
1	F	275	LEU
1	F	322	GLN
1	F	331	GLU
1	F	347	LEU
1	F	356	MET
1	F	390	PHE
1	F	402	ASN
1	F	412	ILE
1	F	419	ARG
1	F	424	VAL
1	F	434	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN

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Mol	Chain	Res	Type
1	A	114	GLN
1	A	142	HIS
1	A	378	GLN
1	A	383	GLN
1	A	433	HIS
1	B	67	ASN
1	B	98	ASN
1	B	242	HIS
1	B	378	GLN
1	B	418	GLN
1	C	67	ASN
1	C	98	ASN
1	C	114	GLN
1	C	142	HIS
1	C	418	GLN
1	D	67	ASN
1	D	162	GLN
1	D	242	HIS
1	D	352	HIS
1	D	378	GLN
1	D	418	GLN
1	D	433	HIS
1	E	67	ASN
1	E	142	HIS
1	E	352	HIS
1	E	378	GLN
1	F	67	ASN
1	F	98	ASN
1	F	142	HIS
1	F	322	GLN
1	F	383	GLN
1	F	418	GLN
1	F	436	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 6 ligands modelled in this entry, 6 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.

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, 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	436/448 (97%)	0.06	19 (4%) 33 29	22, 38, 54, 77	0
1	B	437/448 (97%)	-0.19	9 (2%) 60 58	28, 37, 52, 66	0
1	C	435/448 (97%)	1.07	83 (19%) 2 1	22, 39, 51, 74	0
1	D	436/448 (97%)	0.02	25 (5%) 23 19	26, 38, 53, 70	0
1	E	436/448 (97%)	-0.27	9 (2%) 60 58	25, 37, 47, 68	0
1	F	436/448 (97%)	-0.31	2 (0%) 88 90	26, 37, 48, 64	0
All	All	2616/2688 (97%)	0.06	147 (5%) 24 20	22, 37, 52, 77	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	322	GLN	6.8
1	C	158	THR	6.7
1	C	402	ASN	6.5
1	C	156	CYS	6.2
1	A	157	GLY	5.8
1	C	322	GLN	5.4
1	A	325	THR	5.3
1	C	159	ASP	5.1
1	C	111	LYS	4.9
1	E	322	GLN	4.8
1	A	111	LYS	4.7
1	C	400	THR	4.7
1	C	43	ASP	4.7
1	C	327	LYS	4.6
1	C	206	LEU	4.6
1	C	157	GLY	4.4
1	D	43	ASP	4.4
1	C	38	GLY	4.2
1	C	334	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	38	GLY	4.1
1	C	100	ASN	4.1
1	D	199	ILE	4.1
1	C	325	THR	4.1
1	D	202	GLU	4.0
1	C	403	ALA	4.0
1	C	113	ARG	3.9
1	C	328	THR	3.9
1	C	21	ARG	3.8
1	C	411	PRO	3.8
1	C	122	VAL	3.7
1	A	321	PRO	3.7
1	C	31	VAL	3.7
1	A	204	GLN	3.7
1	C	70	GLY	3.6
1	A	160	ASP	3.6
1	C	4	PHE	3.6
1	C	412	ILE	3.5
1	D	159	ASP	3.5
1	A	43	ASP	3.4
1	A	327	LYS	3.4
1	D	201	ILE	3.4
1	D	404	SER	3.4
1	E	157	GLY	3.4
1	C	205	ARG	3.3
1	C	210	ASP	3.3
1	C	375	LEU	3.3
1	C	114	GLN	3.2
1	C	416	VAL	3.2
1	D	327	LYS	3.2
1	C	203	GLU	3.2
1	D	326	GLY	3.2
1	E	325	THR	3.1
1	C	401	LEU	3.1
1	E	159	ASP	3.1
1	C	101	PRO	3.1
1	C	195	ALA	3.1
1	C	155	GLU	3.1
1	B	322	GLN	3.1
1	D	160	ASP	3.0
1	C	204	GLN	3.0
1	C	115	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	10	SER	3.0
1	D	207	THR	3.0
1	C	355	LYS	2.9
1	A	159	ASP	2.9
1	E	402	ASN	2.9
1	C	32	SER	2.9
1	A	158	THR	2.9
1	C	241	CYS	2.9
1	C	109	LEU	2.9
1	C	130	LEU	2.8
1	C	37	PRO	2.8
1	B	156	CYS	2.8
1	C	199	ILE	2.8
1	D	21	ARG	2.8
1	C	28	ASN	2.8
1	C	3	ARG	2.8
1	D	325	THR	2.8
1	B	43	ASP	2.7
1	C	431	GLY	2.7
1	C	30	ILE	2.7
1	B	158	THR	2.7
1	C	299	ASP	2.7
1	C	137	HIS	2.7
1	D	321	PRO	2.6
1	B	2	LYS	2.6
1	C	141	LEU	2.6
1	C	144	GLY	2.6
1	C	326	GLY	2.5
1	C	162	GLN	2.5
1	C	126	PHE	2.5
1	D	400	THR	2.5
1	C	429	CYS	2.5
1	C	41	SER	2.5
1	A	162	GLN	2.5
1	C	200	ALA	2.5
1	C	186	HIS	2.5
1	B	202	GLU	2.5
1	D	70	GLY	2.4
1	F	43	ASP	2.4
1	A	199	ILE	2.4
1	D	203	GLU	2.4
1	C	276	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	172	GLY	2.4
1	D	205	ARG	2.4
1	D	330	PHE	2.4
1	C	353	LYS	2.4
1	E	43	ASP	2.3
1	C	179	LEU	2.3
1	C	45	GLY	2.3
1	C	121	LEU	2.3
1	F	159	ASP	2.3
1	A	314	SER	2.3
1	B	325	THR	2.3
1	A	411	PRO	2.3
1	E	160	ASP	2.3
1	C	19	THR	2.2
1	D	328	THR	2.2
1	C	399	TYR	2.2
1	C	160	ASP	2.2
1	C	13	VAL	2.2
1	A	74	TRP	2.2
1	C	339	CYS	2.2
1	A	203	GLU	2.2
1	C	87	GLY	2.2
1	D	322	GLN	2.1
1	C	138	LEU	2.1
1	E	204	GLN	2.1
1	C	319	SER	2.1
1	C	283	TYR	2.1
1	C	340	GLN	2.1
1	A	406	LEU	2.1
1	C	15	THR	2.1
1	E	158	THR	2.1
1	C	337	ALA	2.1
1	C	42	SER	2.1
1	D	37	PRO	2.1
1	D	44	ASP	2.1
1	C	63	HIS	2.1
1	B	201	ILE	2.1
1	C	55	LEU	2.1
1	C	335	GLY	2.1
1	D	206	LEU	2.1
1	B	160	ASP	2.0
1	C	145	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	403	ALA	2.0
1	A	101	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ZN	F	447	1/1	0.38	4.28	39,39,39,39	1
2	ZN	E	447	1/1	0.29	2.19	39,39,39,39	1
2	ZN	D	447	1/1	0.28	1.57	40,40,40,40	1
2	ZN	B	447	1/1	0.23	0.81	39,39,39,39	1
2	ZN	A	447	1/1	0.18	-1.26	43,43,43,43	1
2	ZN	C	447	1/1	0.16	-3.13	50,50,50,50	1

6.5 Other polymers ⓘ

There are no such residues in this entry.