



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:19 PM GMT

PDB ID : 4OID
Title : Structural and kinetic bases for the metal preference of the M18 aminopeptidase from *Pseudomonas aeruginosa*
Authors : Nguyen, D.D.; Pandian, R.; Kim, D.D.; Ha, S.C.; Yoon, H.J.; Kim, K.S.; Yun, K.H.; Kim, J.H.; Kim, K.K.
Deposited on : 2014-01-19
Resolution : 2.30 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

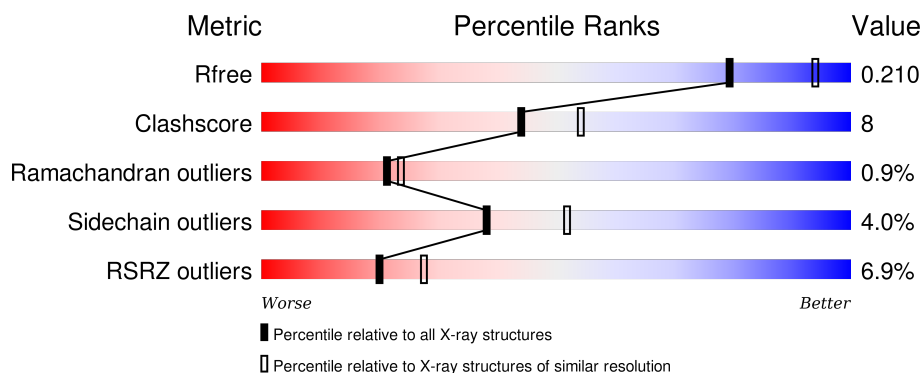
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	429	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>• 5%</div> </div> </div>
1	B	429	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>•• 5%</div> </div> </div>
1	C	429	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	D	429	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13228 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 Probable M18 family aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3151	1979	577	587	8			
1	B	407	Total	C	N	O	S	0	0	0
			3152	1978	578	588	8			
1	C	407	Total	C	N	O	S	0	0	0
			3153	1979	578	588	8			
1	D	407	Total	C	N	O	S	0	0	0
			3153	1979	578	588	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	ASP	ENGINEERED MUTATION	UNP Q9HYZ3
B	236	ALA	ASP	ENGINEERED MUTATION	UNP Q9HYZ3
C	236	ALA	ASP	ENGINEERED MUTATION	UNP Q9HYZ3
D	236	ALA	ASP	ENGINEERED MUTATION	UNP Q9HYZ3

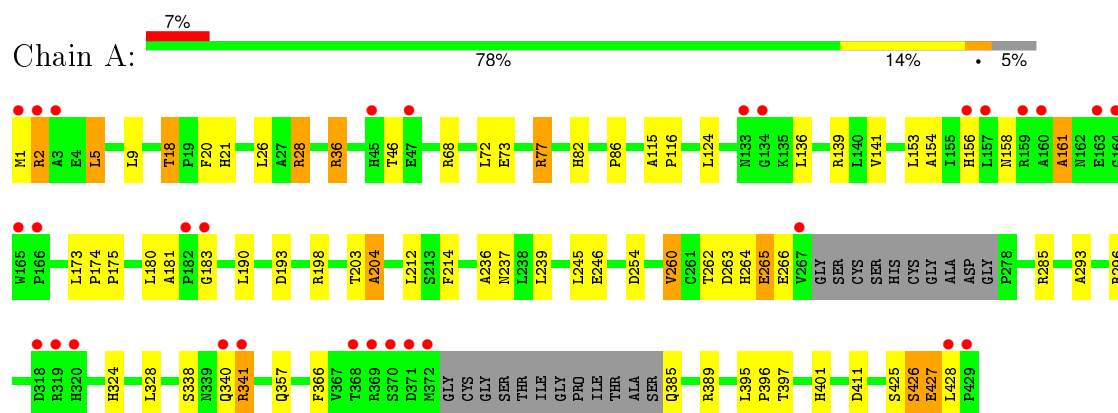
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	146	Total	O	0	0
			146	146		
2	B	167	Total	O	0	0
			167	167		
2	C	153	Total	O	0	0
			153	153		
2	D	153	Total	O	0	0
			153	153		

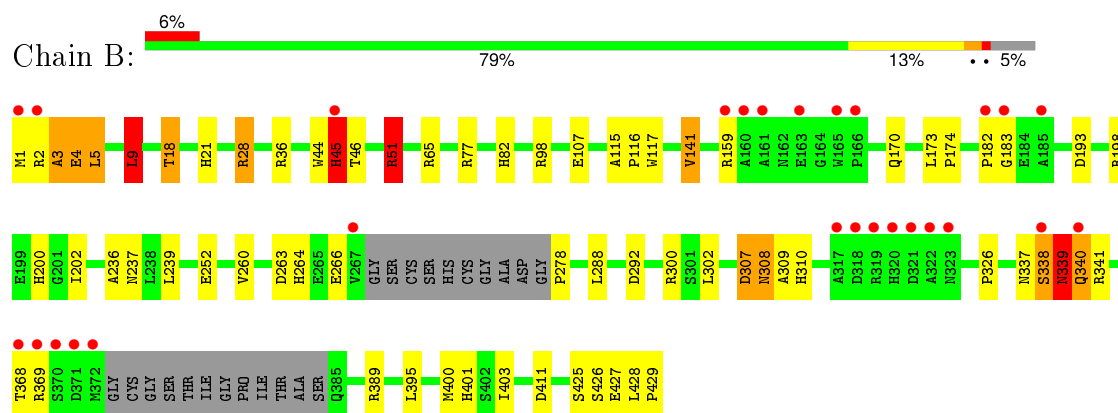
3 Residue-property plots [i](#)

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

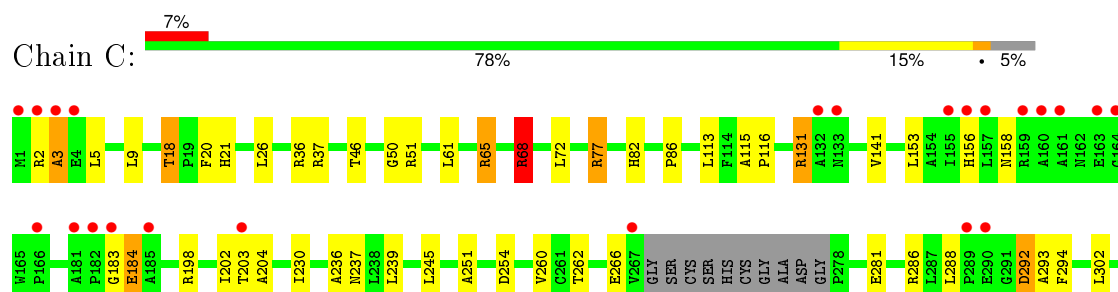
- Molecule 1: Probable M18 family aminopeptidase 2

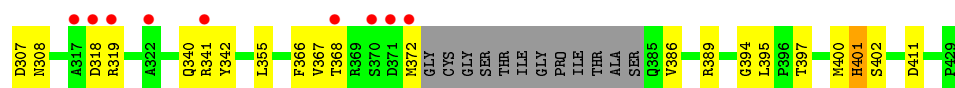


- Molecule 1: Probable M18 family aminopeptidase 2

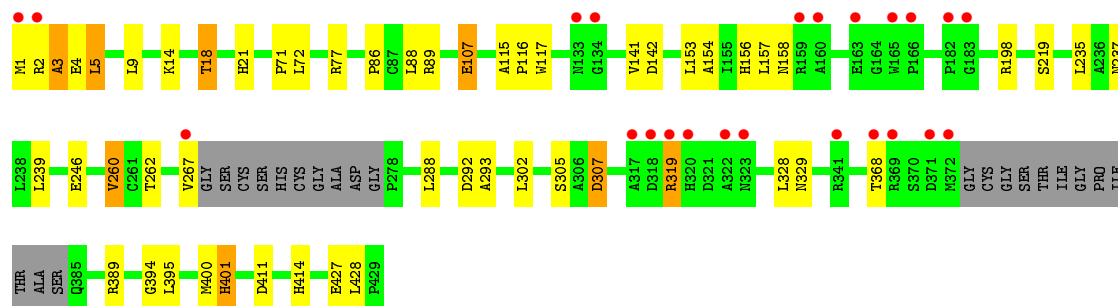
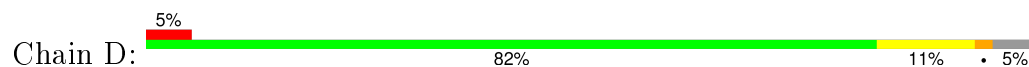


- Molecule 1: Probable M18 family aminopeptidase 2





- Molecule 1: Probable M18 family aminopeptidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	133.61Å 133.61Å 320.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.88 – 2.30 31.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.5 (31.88-2.30) 98.5 (31.88-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.23 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.157 , 0.207 0.162 , 0.210	Depositor DCC
R_{free} test set	4678 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.2	EDS
Estimated twinning fraction	0.012 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.014 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.019 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.008 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.018 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k-1/3*l,4/3*h-4/3*k-1/3*l 0.012 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.030 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 93257 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13228	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.96	0/3215	1.02	7/4361 (0.2%)
1	B	0.98	1/3217 (0.0%)	1.06	13/4366 (0.3%)
1	C	0.94	2/3218 (0.1%)	1.08	19/4368 (0.4%)
1	D	0.96	1/3218 (0.0%)	1.03	8/4368 (0.2%)
All	All	0.96	4/12868 (0.0%)	1.05	47/17463 (0.3%)

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
1	B	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	51	ARG	N-CA	6.54	1.59	1.46
1	C	401	HIS	N-CA	-5.31	1.35	1.46
1	D	305	SER	CB-OG	-5.12	1.35	1.42
1	B	107	GLU	CD-OE2	5.09	1.31	1.25

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	D	77	ARG	NE-CZ-NH2	-12.21	114.20	120.30
1	B	51	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	C	77	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	C	68	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	341	ARG	NE-CZ-NH2	8.10	124.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	400	MET	C-N-CA	7.57	140.64	121.70
1	D	77	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	65	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	B	51	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	400	MET	O-C-N	-6.59	112.16	122.70
1	C	400	MET	O-C-N	-6.45	112.38	122.70
1	C	36	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	401	HIS	N-CA-CB	-6.40	99.09	110.60
1	D	401	HIS	N-CA-CB	-6.35	99.18	110.60
1	B	338	SER	N-CA-C	6.34	128.13	111.00
1	C	50	GLY	N-CA-C	6.33	128.94	113.10
1	A	198	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	68	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	C	65	ARG	CB-CG-CD	-6.05	95.87	111.60
1	B	9	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	B	65	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	254	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	28	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	D	319	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	230	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	C	37	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	A	183	GLY	N-CA-C	-5.50	99.35	113.10
1	D	142	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	260	VAL	CB-CA-C	-5.36	101.21	111.40
1	C	400	MET	C-N-CA	5.34	135.06	121.70
1	B	65	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	286	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	260	VAL	CB-CA-C	-5.27	101.39	111.40
1	B	28	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	292	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	65	ARG	CB-CA-C	-5.25	99.91	110.40
1	B	193	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	98	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	182	PRO	N-CA-C	5.21	125.64	112.10
1	A	36	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	139	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	36	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	260	VAL	CB-CA-C	-5.07	101.76	111.40
1	C	51	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	B	292	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	141	VAL	CG1-CB-CG2	5.00	118.90	110.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	LEU	Peptide
1	A	425	SER	Peptide
1	B	183	GLY	Peptide
1	B	45	HIS	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	3151	0	3094	50	0
1	B	3152	0	3092	60	0
1	C	3153	0	3095	47	0
1	D	3153	0	3095	48	0
2	A	146	0	0	7	0
2	B	167	0	0	11	0
2	C	153	0	0	5	0
2	D	153	0	0	5	0
All	All	13228	0	12376	200	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 8.

All (200) 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:2:ARG:HB3	1:C:3:ALA:CB	1.65	1.26
1:C:2:ARG:CB	1:C:3:ALA:HB3	1.68	1.22
1:B:77:ARG:NH1	1:B:425:SER:O	1.82	1.13
1:B:2:ARG:HB3	1:B:3:ALA:HB3	1.11	1.09
1:D:368:THR:HG23	2:D:697:HOH:O	1.60	1.01
1:B:338:SER:N	1:B:339:ASN:HB2	1.78	0.98
1:C:65:ARG:NH2	1:C:251:ALA:HB3	1.80	0.97
1:B:278:PRO:N	2:B:740:HOH:O	1.98	0.96
1:B:44:TRP:HA	1:B:45:HIS:HB2	1.46	0.94
1:D:2:ARG:HB3	1:D:3:ALA:HB3	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:ARG:HB3	1:B:3:ALA:CB	2.00	0.90
1:A:266:GLU:OE1	2:A:517:HOH:O	1.90	0.89
1:B:337:ASN:C	1:B:339:ASN:HB2	1.93	0.88
1:C:18:THR:HG22	1:C:21:HIS:H	1.40	0.87
1:C:266:GLU:OE1	2:C:515:HOH:O	1.92	0.86
1:A:340:GLN:HG3	1:A:341:ARG:CA	2.08	0.84
1:B:266:GLU:OE1	2:B:622:HOH:O	1.95	0.84
1:B:2:ARG:CB	1:B:3:ALA:HB3	2.02	0.83
1:D:307:ASP:O	1:D:394:GLY:HA2	1.79	0.83
1:A:18:THR:HG22	1:A:21:HIS:H	1.46	0.80
1:C:82:HIS:H	1:C:237:ASN:HD22	1.31	0.79
1:B:338:SER:CA	1:B:339:ASN:OD1	2.32	0.77
1:B:18:THR:HG22	1:B:21:HIS:H	1.49	0.77
1:B:338:SER:N	1:B:339:ASN:CB	2.47	0.77
1:D:88:LEU:HD23	1:D:117:TRP:CE3	2.21	0.75
1:B:1:MET:HB3	1:B:5:LEU:HD22	1.68	0.74
1:D:18:THR:HG22	1:D:21:HIS:H	1.53	0.73
1:A:153:LEU:HD23	1:A:158:ASN:HB2	1.69	0.73
1:C:236:ALA:HB2	1:C:308:ASN:HD22	1.54	0.72
1:A:395:LEU:HD22	1:A:411:ASP:HB3	1.72	0.71
1:B:337:ASN:ND2	1:B:340:GLN:NE2	2.39	0.71
1:B:278:PRO:CD	2:B:740:HOH:O	2.38	0.70
1:A:72:LEU:HD21	1:A:293:ALA:HB1	1.72	0.70
1:B:82:HIS:H	1:B:237:ASN:HD22	1.38	0.69
1:B:2:ARG:HB2	1:B:4:GLU:H	1.58	0.68
1:B:338:SER:C	1:B:339:ASN:OD1	2.32	0.68
1:D:302:LEU:HD12	1:D:389:ARG:O	1.93	0.68
1:A:389:ARG:HH22	1:A:428:LEU:HD21	1.59	0.66
1:B:339:ASN:O	1:B:340:GLN:OE1	2.14	0.66
1:B:44:TRP:HA	1:B:45:HIS:CB	2.22	0.66
1:D:368:THR:N	2:D:697:HOH:O	2.15	0.65
1:A:82:HIS:H	1:A:237:ASN:HD22	1.44	0.65
1:D:2:ARG:HB2	1:D:4:GLU:H	1.61	0.65
1:A:385:GLN:HA	1:A:385:GLN:OE1	1.95	0.65
1:B:337:ASN:HD21	1:B:340:GLN:NE2	1.96	0.64
1:A:401:HIS:NE2	2:A:517:HOH:O	2.30	0.64
1:B:341:ARG:NH2	2:B:698:HOH:O	2.27	0.63
1:B:428:LEU:HB3	1:B:429:PRO:HD2	1.79	0.63
1:B:44:TRP:CA	1:B:45:HIS:HB2	2.27	0.62
1:B:1:MET:CB	1:B:5:LEU:HD22	2.28	0.62
1:A:82:HIS:CE1	1:A:237:ASN:HB2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PRO:HG2	1:D:401:HIS:CG	2.36	0.61
1:B:309:ALA:HB1	2:B:746:HOH:O	2.00	0.60
1:D:427:GLU:O	1:D:428:LEU:HD23	2.02	0.60
1:C:401:HIS:CE1	1:D:156:HIS:CE1	2.89	0.60
1:A:158:ASN:O	1:A:161:ALA:HB2	2.04	0.58
1:C:395:LEU:HD22	1:C:411:ASP:HB3	1.85	0.58
1:B:338:SER:CB	1:B:339:ASN:OD1	2.51	0.58
1:C:203:THR:O	1:C:203:THR:HG22	2.02	0.58
1:D:267:VAL:HG12	1:D:267:VAL:O	2.04	0.58
1:B:51:ARG:HD3	2:B:668:HOH:O	2.04	0.57
1:A:264:HIS:C	1:A:265:GLU:O	2.38	0.57
1:B:338:SER:N	1:B:339:ASN:CG	2.59	0.56
1:C:9:LEU:HD22	1:C:239:LEU:HD12	1.88	0.56
1:C:386:VAL:O	1:C:386:VAL:HG12	2.06	0.55
1:D:153:LEU:HD23	1:D:158:ASN:HB2	1.87	0.55
1:D:267:VAL:CG1	1:D:267:VAL:O	2.54	0.55
1:D:198:ARG:NH1	2:D:740:HOH:O	2.39	0.55
1:C:86:PRO:HG2	1:C:401:HIS:CG	2.42	0.55
1:D:2:ARG:CB	1:D:4:GLU:H	2.20	0.54
1:B:2:ARG:CB	1:B:4:GLU:H	2.19	0.54
1:C:72:LEU:HD11	1:C:293:ALA:HB1	1.90	0.54
1:C:198:ARG:NH1	2:C:617:HOH:O	2.41	0.54
1:C:307:ASP:O	1:C:394:GLY:CA	2.56	0.54
1:B:28:ARG:NH2	2:B:690:HOH:O	2.34	0.54
1:C:319:ARG:NH1	1:D:157:LEU:O	2.41	0.53
1:B:338:SER:OG	1:B:339:ASN:OD1	2.25	0.53
1:A:77:ARG:NH2	1:A:427:GLU:HG2	2.24	0.53
1:A:340:GLN:CG	1:A:341:ARG:CA	2.85	0.53
1:D:237:ASN:HD21	1:D:307:ASP:HA	1.73	0.53
1:D:2:ARG:NH2	1:D:2:ARG:HA	2.24	0.52
1:A:68:ARG:HB3	1:A:254:ASP:OD2	2.09	0.52
1:A:72:LEU:HD21	1:A:293:ALA:CB	2.39	0.52
1:D:427:GLU:C	1:D:428:LEU:HD23	2.30	0.52
1:C:236:ALA:HB2	1:C:308:ASN:ND2	2.23	0.52
1:C:307:ASP:O	1:C:394:GLY:HA2	2.10	0.52
1:A:26:LEU:HD23	1:A:245:LEU:HD22	1.93	0.51
1:D:1:MET:O	1:D:5:LEU:HB2	2.09	0.51
1:D:72:LEU:HD11	1:D:293:ALA:HA	1.91	0.51
2:C:530:HOH:O	1:D:154:ALA:HB2	2.11	0.51
1:A:154:ALA:HB2	2:B:661:HOH:O	2.11	0.51
1:A:328:LEU:HD12	1:A:396:PRO:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:PRO:HG2	1:A:401:HIS:CG	2.46	0.50
1:A:9:LEU:CD2	1:A:239:LEU:HD13	2.41	0.50
1:B:340:GLN:HA	1:B:340:GLN:OE1	2.10	0.50
1:B:44:TRP:CA	1:B:45:HIS:CB	2.88	0.50
1:D:88:LEU:CD2	1:D:117:TRP:CD2	2.95	0.50
1:A:296:ARG:NH2	2:A:591:HOH:O	2.31	0.49
1:B:1:MET:O	1:B:5:LEU:HB2	2.11	0.49
1:D:88:LEU:HD23	1:D:117:TRP:CZ3	2.47	0.49
1:B:2:ARG:NE	1:B:2:ARG:HA	2.27	0.49
1:D:2:ARG:CB	1:D:3:ALA:HB3	2.32	0.49
1:C:2:ARG:HB3	1:C:3:ALA:HB3	0.72	0.49
1:A:72:LEU:CD2	1:A:293:ALA:O	2.60	0.49
1:D:328:LEU:O	1:D:329:ASN:HB2	2.11	0.49
1:D:88:LEU:N	1:D:88:LEU:HD22	2.28	0.48
1:C:288:LEU:HD13	1:C:294:PHE:HA	1.94	0.48
1:C:366:PHE:CE1	1:C:368:THR:HG22	2.47	0.48
1:D:71:PRO:HB2	1:D:288:LEU:HD21	1.94	0.48
1:D:395:LEU:HD22	1:D:411:ASP:HB3	1.95	0.48
1:B:117:TRP:CD2	1:B:403:ILE:HD12	2.49	0.48
1:C:239:LEU:HD21	1:C:395:LEU:HD12	1.95	0.48
1:B:115:ALA:N	1:B:116:PRO:CD	2.76	0.48
1:B:170:GLN:NE2	2:B:745:HOH:O	2.40	0.48
1:C:260:VAL:HG12	1:C:262:THR:HG23	1.95	0.48
1:D:88:LEU:CD2	1:D:117:TRP:CE3	2.95	0.48
1:A:389:ARG:NH2	1:A:428:LEU:HD11	2.28	0.47
1:A:28:ARG:NH2	2:A:612:HOH:O	2.45	0.47
1:B:263:ASP:OD1	1:B:264:HIS:N	2.47	0.47
1:D:260:VAL:HG12	1:D:262:THR:HG23	1.96	0.47
1:B:236:ALA:HB2	1:B:308:ASN:HD22	1.79	0.47
1:C:341:ARG:HG3	1:C:342:TYR:CD2	2.49	0.47
1:A:72:LEU:HD21	1:A:293:ALA:CA	2.45	0.47
1:C:153:LEU:HD23	1:C:158:ASN:HB2	1.96	0.47
1:B:337:ASN:ND2	1:B:340:GLN:HE21	2.11	0.46
1:D:2:ARG:HB2	1:D:4:GLU:N	2.30	0.46
1:A:260:VAL:HG12	1:A:262:THR:HG23	1.96	0.46
1:A:72:LEU:HD21	1:A:293:ALA:O	2.14	0.46
1:B:9:LEU:CD1	1:B:239:LEU:HD13	2.45	0.46
1:B:173:LEU:N	1:B:174:PRO:CD	2.78	0.46
1:A:340:GLN:HE21	1:A:340:GLN:H	1.63	0.46
1:B:117:TRP:CE3	1:B:403:ILE:HD12	2.50	0.46
1:D:9:LEU:HD22	1:D:239:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:HG3	1:C:386:VAL:HG13	1.97	0.46
1:D:9:LEU:CD2	1:D:239:LEU:HD13	2.46	0.46
1:C:18:THR:HG23	1:C:20:PHE:H	1.81	0.46
1:B:300:ARG:O	1:B:428:LEU:HD12	2.15	0.45
1:B:338:SER:CA	1:B:339:ASN:CG	2.85	0.45
1:C:302:LEU:HD12	1:C:389:ARG:O	2.17	0.45
1:C:307:ASP:O	1:C:394:GLY:HA3	2.17	0.45
1:A:68:ARG:N	1:A:254:ASP:OD2	2.50	0.45
1:A:193:ASP:OD1	1:A:204:ALA:HB3	2.16	0.45
1:C:82:HIS:N	1:C:237:ASN:HD22	2.07	0.45
1:A:18:THR:HG23	1:A:20:PHE:H	1.81	0.45
1:A:236:ALA:HA	1:A:237:ASN:HA	1.72	0.44
1:D:9:LEU:HD21	1:D:239:LEU:HD13	2.00	0.44
1:D:72:LEU:HA	1:D:72:LEU:HD12	1.65	0.44
1:A:203:THR:O	1:A:204:ALA:HB3	2.17	0.44
1:B:400:MET:O	1:B:401:HIS:HB2	2.17	0.44
1:B:200:HIS:HB2	1:B:202:ILE:HD12	1.99	0.44
1:D:389:ARG:NH2	2:D:720:HOH:O	2.49	0.44
1:C:68:ARG:HH11	1:C:68:ARG:HG3	1.83	0.44
1:C:292:ASP:HA	2:C:582:HOH:O	2.17	0.44
1:A:324:HIS:HB3	1:A:366:PHE:HA	1.98	0.44
1:B:389:ARG:HG3	2:B:637:HOH:O	2.18	0.44
1:D:5:LEU:HD11	1:D:246:GLU:HG2	1.99	0.44
1:B:288:LEU:HA	1:B:288:LEU:HD23	1.74	0.44
1:C:82:HIS:CE1	1:C:237:ASN:HB2	2.53	0.43
1:D:414:HIS:HE1	2:D:702:HOH:O	2.01	0.43
1:A:285:ARG:NH2	2:A:606:HOH:O	2.51	0.43
1:C:115:ALA:N	1:C:116:PRO:CD	2.80	0.43
1:A:263:ASP:OD1	1:A:264:HIS:N	2.50	0.43
1:D:292:ASP:O	1:D:293:ALA:C	2.57	0.43
1:C:131:ARG:NH2	2:C:598:HOH:O	2.50	0.43
1:C:239:LEU:CD2	1:C:395:LEU:HD12	2.48	0.43
1:C:153:LEU:HD21	1:D:319:ARG:HG3	2.00	0.43
1:D:115:ALA:N	1:D:116:PRO:HD2	2.34	0.43
1:B:302:LEU:HB2	1:B:428:LEU:HD13	2.01	0.43
1:A:5:LEU:HD11	1:A:246:GLU:HG2	2.01	0.43
1:C:203:THR:CG2	1:C:203:THR:O	2.67	0.43
1:C:2:ARG:HB3	1:C:3:ALA:CA	2.43	0.42
1:A:82:HIS:H	1:A:237:ASN:ND2	2.14	0.42
1:B:237:ASN:OD1	1:B:307:ASP:HA	2.19	0.42
1:D:89:ARG:HB2	1:D:107:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ALA:HA	1:B:237:ASN:HA	1.68	0.42
1:C:156:HIS:CE1	1:D:401:HIS:CE1	3.08	0.42
1:C:113:LEU:HD12	1:C:402:SER:N	2.34	0.42
1:A:115:ALA:N	1:A:116:PRO:CD	2.82	0.42
1:C:26:LEU:HD23	1:C:245:LEU:HD22	2.01	0.42
1:C:236:ALA:HA	1:C:237:ASN:HA	1.76	0.41
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.82	0.41
1:A:426:SER:HA	1:A:427:GLU:HA	1.82	0.41
1:B:395:LEU:HD13	1:B:411:ASP:HB3	2.01	0.41
1:A:36:ARG:NH2	2:A:590:HOH:O	2.53	0.41
1:A:124:LEU:HD13	1:A:214:PHE:CE1	2.56	0.41
1:B:9:LEU:HD11	1:B:239:LEU:HD13	2.01	0.41
1:B:200:HIS:CB	1:B:202:ILE:HD12	2.50	0.41
1:C:61:LEU:C	1:C:61:LEU:HD23	2.41	0.41
1:D:2:ARG:CZ	1:D:2:ARG:HA	2.51	0.41
1:D:307:ASP:O	1:D:394:GLY:CA	2.60	0.41
1:A:173:LEU:N	1:A:174:PRO:CD	2.84	0.41
1:B:338:SER:H	1:B:339:ASN:CG	2.24	0.41
1:A:174:PRO:HA	1:A:175:PRO:HD3	1.92	0.41
1:B:28:ARG:HD2	2:B:767:HOH:O	2.21	0.40
1:A:124:LEU:HD13	1:A:214:PHE:CD1	2.56	0.40
1:A:156:HIS:HB2	1:B:310:HIS:CE1	2.57	0.40
1:A:357:GLN:NE2	2:A:625:HOH:O	2.55	0.40
1:D:14:LYS:HE2	1:D:219:SER:OG	2.22	0.40
1:C:65:ARG:HH22	1:C:251:ALA:HB3	1.77	0.40
1:C:183:GLY:HA3	1:C:184:GLU:CB	2.52	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	399/429 (93%)	373 (94%)	21 (5%)	5 (1%)	15	15
1	B	401/429 (94%)	373 (93%)	22 (6%)	6 (2%)	13	12
1	C	401/429 (94%)	376 (94%)	22 (6%)	3 (1%)	26	31
1	D	401/429 (94%)	382 (95%)	18 (4%)	1 (0%)	52	64
All	All	1602/1716 (93%)	1504 (94%)	83 (5%)	15 (1%)	21	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	ALA
1	B	3	ALA
1	B	369	ARG
1	C	3	ALA
1	C	184	GLU
1	C	204	ALA
1	D	3	ALA
1	A	161	ALA
1	B	45	HIS
1	B	339	ASN
1	B	308	ASN
1	A	2	ARG
1	A	204	ALA
1	B	368	THR
1	A	265	GLU

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	328/343 (96%)	313 (95%)	15 (5%)	33	44
1	B	329/343 (96%)	312 (95%)	17 (5%)	29	38
1	C	329/343 (96%)	315 (96%)	14 (4%)	35	47
1	D	329/343 (96%)	323 (98%)	6 (2%)	66	82
All	All	1315/1372 (96%)	1263 (96%)	52 (4%)	38	52

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	5	LEU
1	A	18	THR
1	A	46	THR
1	A	73	GLU
1	A	77	ARG
1	A	136	LEU
1	A	141	VAL
1	A	190	LEU
1	A	212	LEU
1	A	338	SER
1	A	397	THR
1	A	426	SER
1	A	427	GLU
1	B	4	GLU
1	B	5	LEU
1	B	9	LEU
1	B	18	THR
1	B	36	ARG
1	B	46	THR
1	B	51	ARG
1	B	141	VAL
1	B	159	ARG
1	B	198	ARG
1	B	252	GLU
1	B	307	ASP
1	B	326	PRO
1	B	339	ASN
1	B	340	GLN
1	B	426	SER
1	B	427	GLU
1	C	5	LEU
1	C	18	THR
1	C	46	THR
1	C	68	ARG
1	C	77	ARG
1	C	131	ARG
1	C	141	VAL
1	C	202	ILE
1	C	318	ASP
1	C	340	GLN

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Mol	Chain	Res	Type
1	C	355	LEU
1	C	367	VAL
1	C	372	MET
1	C	397	THR
1	D	5	LEU
1	D	18	THR
1	D	107	GLU
1	D	141	VAL
1	D	235	LEU
1	D	307	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	237	ASN
1	B	308	ASN
1	B	340	GLN
1	B	357	GLN
1	C	156	HIS
1	C	237	ASN
1	C	308	ASN
1	D	237	ASN
1	D	414	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

There are no ligands in this entry.

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	407/429 (94%)	-0.12	30 (7%) 17 25	14, 25, 66, 97	0
1	B	407/429 (94%)	-0.18	27 (6%) 22 29	13, 25, 65, 96	0
1	C	407/429 (94%)	-0.12	32 (7%) 15 22	13, 25, 62, 111	0
1	D	407/429 (94%)	-0.16	23 (5%) 27 36	13, 25, 61, 96	0
All	All	1628/1716 (94%)	-0.14	112 (6%) 20 27	13, 25, 64, 111	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	8.8
1	B	372	MET	8.5
1	C	372	MET	7.9
1	D	372	MET	7.9
1	C	159	ARG	6.8
1	B	1	MET	5.8
1	C	160	ALA	5.6
1	D	1	MET	5.4
1	A	428	LEU	5.3
1	A	165	TRP	5.3
1	D	318	ASP	5.1
1	D	159	ARG	5.1
1	A	372	MET	5.0
1	A	163	GLU	4.9
1	A	159	ARG	4.9
1	A	160	ALA	4.9
1	B	160	ALA	4.6
1	C	163	GLU	4.5
1	B	159	ARG	4.5
1	C	368	THR	4.4
1	B	368	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	371	ASP	4.3
1	B	318	ASP	4.3
1	A	429	PRO	4.2
1	B	267	VAL	4.0
1	A	182	PRO	3.9
1	D	368	THR	3.9
1	D	160	ALA	3.9
1	D	267	VAL	3.8
1	A	368	THR	3.8
1	A	318	ASP	3.7
1	B	370	SER	3.7
1	B	163	GLU	3.7
1	D	319	ARG	3.6
1	B	371	ASP	3.6
1	C	182	PRO	3.6
1	B	182	PRO	3.6
1	C	2	ARG	3.6
1	B	183	GLY	3.5
1	C	318	ASP	3.5
1	A	166	PRO	3.5
1	A	164	GLY	3.5
1	C	371	ASP	3.5
1	D	163	GLU	3.4
1	C	156	HIS	3.4
1	C	164	GLY	3.3
1	D	323	ASN	3.3
1	D	371	ASP	3.3
1	D	320	HIS	3.3
1	A	2	ARG	3.3
1	A	157	LEU	3.3
1	C	267	VAL	3.2
1	C	181	ALA	3.2
1	B	45	HIS	3.1
1	D	183	GLY	3.1
1	D	182	PRO	3.1
1	A	341	ARG	3.1
1	D	166	PRO	3.0
1	D	322	ALA	3.0
1	C	370	SER	2.9
1	D	134	GLY	2.9
1	B	165	TRP	2.9
1	A	3	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	165	TRP	2.8
1	D	341	ARG	2.8
1	A	183	GLY	2.8
1	C	183	GLY	2.8
1	B	317	ALA	2.7
1	A	267	VAL	2.7
1	B	322	ALA	2.7
1	C	322	ALA	2.7
1	A	319	ARG	2.7
1	C	133	ASN	2.6
1	A	1	MET	2.6
1	D	2	ARG	2.6
1	D	133	ASN	2.6
1	C	289	PRO	2.5
1	A	134	GLY	2.5
1	A	156	HIS	2.5
1	D	317	ALA	2.5
1	B	369	ARG	2.5
1	C	157	LEU	2.5
1	C	3	ALA	2.4
1	C	132	ALA	2.4
1	C	203	THR	2.4
1	C	290	GLU	2.4
1	B	2	ARG	2.4
1	B	166	PRO	2.4
1	B	185	ALA	2.4
1	C	161	ALA	2.4
1	B	323	ASN	2.3
1	C	155	ILE	2.3
1	C	319	ARG	2.3
1	B	340	GLN	2.3
1	C	166	PRO	2.3
1	B	161	ALA	2.3
1	C	185	ALA	2.3
1	A	340	GLN	2.2
1	A	320	HIS	2.2
1	C	317	ALA	2.2
1	B	319	ARG	2.2
1	B	320	HIS	2.2
1	A	45	HIS	2.1
1	A	133	ASN	2.1
1	C	341	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	47	GLU	2.1
1	D	369	ARG	2.1
1	B	338	SER	2.1
1	B	321	ASP	2.0
1	A	370	SER	2.0
1	A	369	ARG	2.0
1	C	4	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.