



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:56 PM UTC

PDB ID : 4IWS / pdb_00004iws
Title : Putative Aromatic Acid Decarboxylase
Authors : Jacewicz, A.; Izumi, A.; Brunner, K.; Schneider, G.
Deposited on : 2013-01-24
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
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

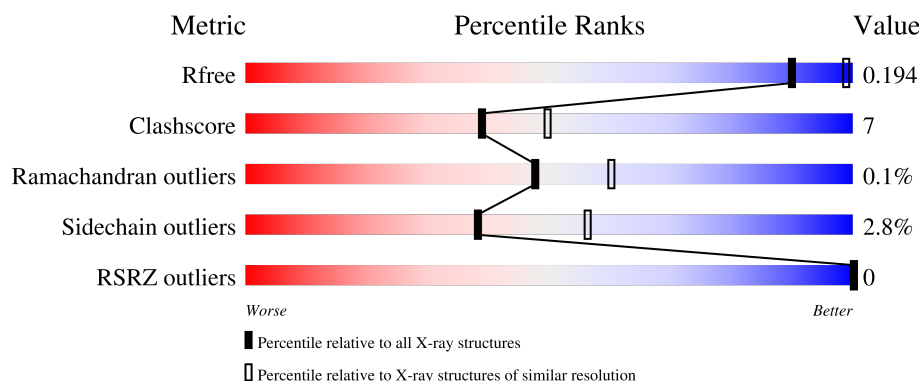
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

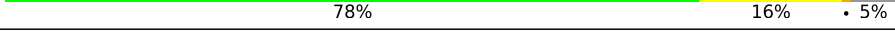
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	518	
1	B	518	
1	C	518	
1	D	518	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15569 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 PA0254.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	11	0	0
			3831	2432	699	685	15			
1	B	495	Total	C	N	O	S	15	0	0
			3840	2436	701	689	14			
1	C	491	Total	C	N	O	S	38	0	0
			3815	2423	696	682	14			
1	D	493	Total	C	N	O	S	40	0	0
			3831	2432	699	685	15			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9I6N5
A	-20	HIS	-	expression tag	UNP Q9I6N5
A	-19	HIS	-	expression tag	UNP Q9I6N5
A	-18	HIS	-	expression tag	UNP Q9I6N5
A	-17	HIS	-	expression tag	UNP Q9I6N5
A	-16	HIS	-	expression tag	UNP Q9I6N5
A	-15	HIS	-	expression tag	UNP Q9I6N5
A	-14	SER	-	expression tag	UNP Q9I6N5
A	-13	SER	-	expression tag	UNP Q9I6N5
A	-12	GLY	-	expression tag	UNP Q9I6N5
A	-11	VAL	-	expression tag	UNP Q9I6N5
A	-10	ASP	-	expression tag	UNP Q9I6N5
A	-9	LEU	-	expression tag	UNP Q9I6N5
A	-8	GLY	-	expression tag	UNP Q9I6N5
A	-7	THR	-	expression tag	UNP Q9I6N5
A	-6	GLU	-	expression tag	UNP Q9I6N5
A	-5	ASN	-	expression tag	UNP Q9I6N5
A	-4	LEU	-	expression tag	UNP Q9I6N5
A	-3	TYR	-	expression tag	UNP Q9I6N5
A	-2	PHE	-	expression tag	UNP Q9I6N5
A	-1	GLN	-	expression tag	UNP Q9I6N5

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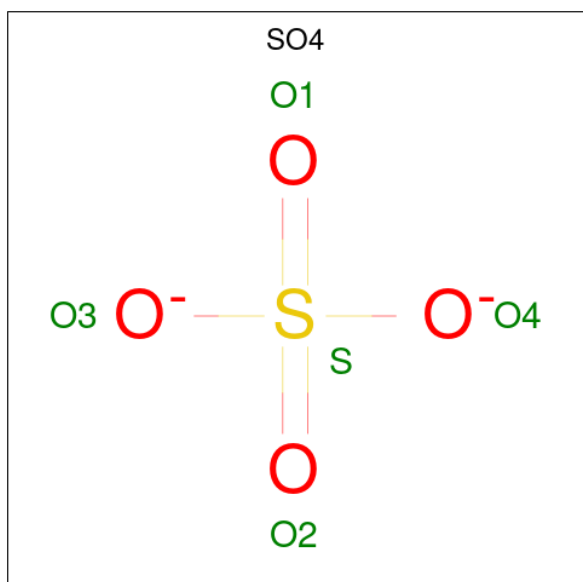
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q9I6N5
B	-21	MET	-	expression tag	UNP Q9I6N5
B	-20	HIS	-	expression tag	UNP Q9I6N5
B	-19	HIS	-	expression tag	UNP Q9I6N5
B	-18	HIS	-	expression tag	UNP Q9I6N5
B	-17	HIS	-	expression tag	UNP Q9I6N5
B	-16	HIS	-	expression tag	UNP Q9I6N5
B	-15	HIS	-	expression tag	UNP Q9I6N5
B	-14	SER	-	expression tag	UNP Q9I6N5
B	-13	SER	-	expression tag	UNP Q9I6N5
B	-12	GLY	-	expression tag	UNP Q9I6N5
B	-11	VAL	-	expression tag	UNP Q9I6N5
B	-10	ASP	-	expression tag	UNP Q9I6N5
B	-9	LEU	-	expression tag	UNP Q9I6N5
B	-8	GLY	-	expression tag	UNP Q9I6N5
B	-7	THR	-	expression tag	UNP Q9I6N5
B	-6	GLU	-	expression tag	UNP Q9I6N5
B	-5	ASN	-	expression tag	UNP Q9I6N5
B	-4	LEU	-	expression tag	UNP Q9I6N5
B	-3	TYR	-	expression tag	UNP Q9I6N5
B	-2	PHE	-	expression tag	UNP Q9I6N5
B	-1	GLN	-	expression tag	UNP Q9I6N5
B	0	SER	-	expression tag	UNP Q9I6N5
C	-21	MET	-	expression tag	UNP Q9I6N5
C	-20	HIS	-	expression tag	UNP Q9I6N5
C	-19	HIS	-	expression tag	UNP Q9I6N5
C	-18	HIS	-	expression tag	UNP Q9I6N5
C	-17	HIS	-	expression tag	UNP Q9I6N5
C	-16	HIS	-	expression tag	UNP Q9I6N5
C	-15	HIS	-	expression tag	UNP Q9I6N5
C	-14	SER	-	expression tag	UNP Q9I6N5
C	-13	SER	-	expression tag	UNP Q9I6N5
C	-12	GLY	-	expression tag	UNP Q9I6N5
C	-11	VAL	-	expression tag	UNP Q9I6N5
C	-10	ASP	-	expression tag	UNP Q9I6N5
C	-9	LEU	-	expression tag	UNP Q9I6N5
C	-8	GLY	-	expression tag	UNP Q9I6N5
C	-7	THR	-	expression tag	UNP Q9I6N5
C	-6	GLU	-	expression tag	UNP Q9I6N5
C	-5	ASN	-	expression tag	UNP Q9I6N5
C	-4	LEU	-	expression tag	UNP Q9I6N5
C	-3	TYR	-	expression tag	UNP Q9I6N5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP Q9I6N5
C	-1	GLN	-	expression tag	UNP Q9I6N5
C	0	SER	-	expression tag	UNP Q9I6N5
D	-21	MET	-	expression tag	UNP Q9I6N5
D	-20	HIS	-	expression tag	UNP Q9I6N5
D	-19	HIS	-	expression tag	UNP Q9I6N5
D	-18	HIS	-	expression tag	UNP Q9I6N5
D	-17	HIS	-	expression tag	UNP Q9I6N5
D	-16	HIS	-	expression tag	UNP Q9I6N5
D	-15	HIS	-	expression tag	UNP Q9I6N5
D	-14	SER	-	expression tag	UNP Q9I6N5
D	-13	SER	-	expression tag	UNP Q9I6N5
D	-12	GLY	-	expression tag	UNP Q9I6N5
D	-11	VAL	-	expression tag	UNP Q9I6N5
D	-10	ASP	-	expression tag	UNP Q9I6N5
D	-9	LEU	-	expression tag	UNP Q9I6N5
D	-8	GLY	-	expression tag	UNP Q9I6N5
D	-7	THR	-	expression tag	UNP Q9I6N5
D	-6	GLU	-	expression tag	UNP Q9I6N5
D	-5	ASN	-	expression tag	UNP Q9I6N5
D	-4	LEU	-	expression tag	UNP Q9I6N5
D	-3	TYR	-	expression tag	UNP Q9I6N5
D	-2	PHE	-	expression tag	UNP Q9I6N5
D	-1	GLN	-	expression tag	UNP Q9I6N5
D	0	SER	-	expression tag	UNP Q9I6N5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

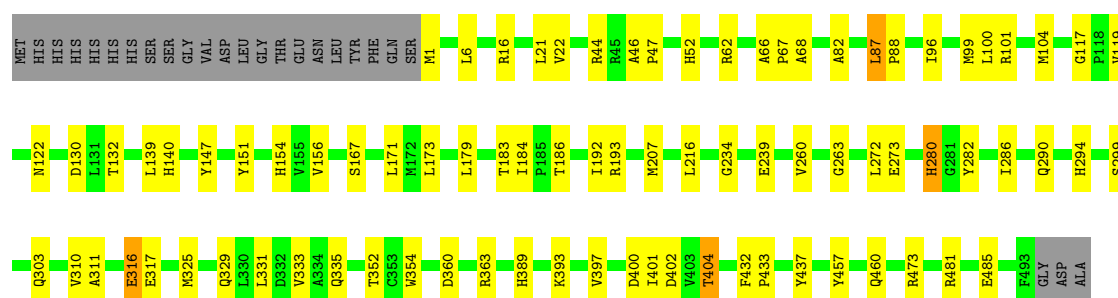
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	77	Total	O		0	0
			77	77			
3	B	68	Total	O		0	0
			68	68			
3	C	53	Total	O		0	0
			53	53			
3	D	49	Total	O		0	0
			49	49			

3 Residue-property plots [i](#)

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.

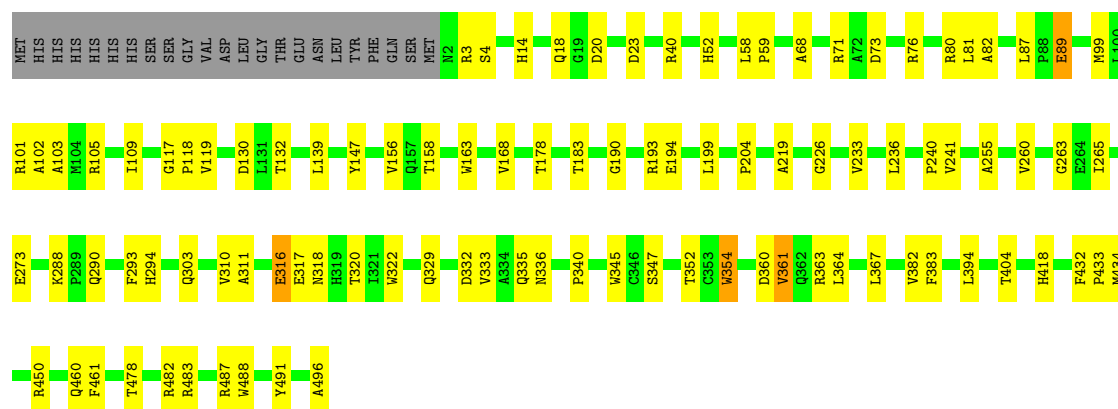
• Molecule 1: PA0254

Chain A: 



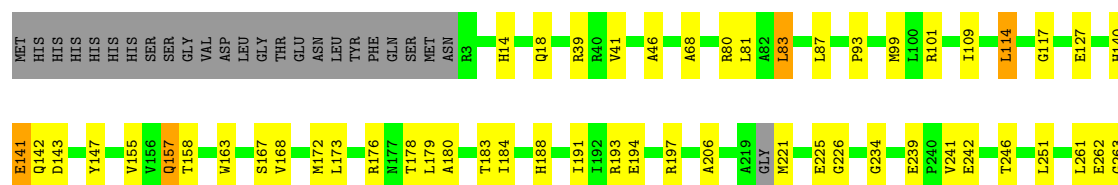
• Molecule 1: PA0254

Chain B: 



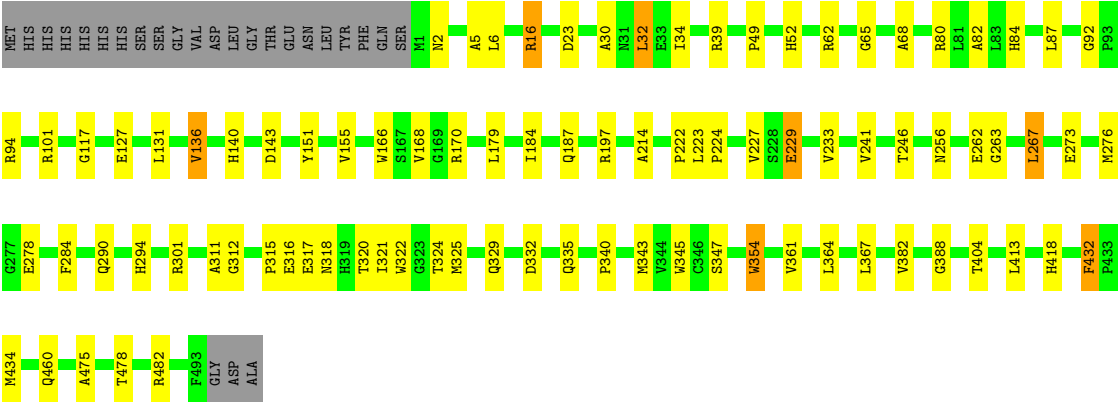
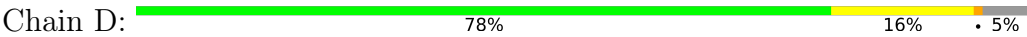
• Molecule 1: PA0254

Chain C: 





• Molecule 1: PA0254



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.30Å 55.82Å 198.42Å 90.00° 90.87° 90.00°	Depositor
Resolution (Å)	49.21 – 2.30 49.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.21-2.30) 94.3 (49.21-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.164 , 0.219 0.163 , 0.194	Depositor DCC
R_{free} test set	5038 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 7.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.200 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15569	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.49	0/3939	0.89	6/5378 (0.1%)
1	B	0.49	0/3948	0.87	5/5391 (0.1%)
1	C	0.48	0/3922	0.88	6/5354 (0.1%)
1	D	0.47	0/3939	0.88	11/5378 (0.2%)
All	All	0.48	0/15748	0.88	28/21501 (0.1%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLY	CA-C-N	6.93	126.54	119.19
1	B	117	GLY	C-N-CA	6.93	126.54	119.19
1	A	87	LEU	CA-C-N	6.83	128.38	119.84
1	A	87	LEU	C-N-CA	6.83	128.38	119.84
1	C	117	GLY	CA-C-N	6.58	126.35	119.05
1	C	117	GLY	C-N-CA	6.58	126.35	119.05
1	D	418	HIS	CA-C-N	6.37	127.80	119.84
1	D	418	HIS	C-N-CA	6.37	127.80	119.84
1	D	354	TRP	N-CA-C	6.14	118.74	109.23
1	B	418	HIS	CA-C-N	6.12	126.58	119.47
1	B	418	HIS	C-N-CA	6.12	126.58	119.47
1	D	432	PHE	CA-C-N	5.87	125.49	119.56
1	D	432	PHE	C-N-CA	5.87	125.49	119.56
1	D	284	PHE	CA-C-N	5.70	125.06	118.85
1	D	284	PHE	C-N-CA	5.70	125.06	118.85
1	C	418	HIS	CA-C-N	5.65	126.90	119.84
1	C	418	HIS	C-N-CA	5.65	126.90	119.84
1	D	117	GLY	CA-C-N	5.62	125.99	119.47
1	D	117	GLY	C-N-CA	5.62	125.99	119.47
1	D	92	GLY	CA-C-N	5.55	126.78	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	92	GLY	C-N-CA	5.55	126.78	119.84
1	C	184	ILE	CA-C-N	5.24	125.55	119.47
1	C	184	ILE	C-N-CA	5.24	125.55	119.47
1	A	117	GLY	CA-C-N	5.21	124.87	119.56
1	A	117	GLY	C-N-CA	5.21	124.87	119.56
1	B	89	GLU	N-CA-C	5.11	118.29	111.75
1	A	184	ILE	CA-C-N	5.07	124.85	119.28
1	A	184	ILE	C-N-CA	5.07	124.85	119.28

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	3831	0	3758	54	0
1	B	3840	0	3758	53	0
1	C	3815	0	3739	51	0
1	D	3831	0	3758	52	0
2	D	5	0	0	0	0
3	A	77	0	0	1	0
3	B	68	0	0	0	0
3	C	53	0	0	2	0
3	D	49	0	0	2	0
All	All	15569	0	15013	206	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 7.

All (206) 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:A:44:ARG:HE	1:B:496:ALA:HB3	1.32	0.90
1:A:62:ARG:NH2	1:A:303:GLN:O	2.20	0.74
1:A:104:MET:HE1	1:A:329:GLN:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:HIS:HD2	1:A:282:TYR:H	1.33	0.73
1:D:197:ARG:NH2	1:D:267:LEU:O	2.25	0.70
1:D:278:GLU:HG3	1:D:434:MET:HE1	1.74	0.69
1:C:183:THR:HG21	1:C:193:ARG:HD3	1.75	0.68
1:B:68:ALA:HB3	1:B:317:GLU:HG3	1.76	0.66
1:B:139:LEU:HD22	1:B:310:VAL:HG22	1.77	0.65
1:A:316:GLU:HG2	1:A:317:GLU:H	1.61	0.65
1:D:94:ARG:HG2	1:D:343:MET:HE3	1.78	0.64
1:A:400:ASP:OD1	3:A:573:HOH:O	2.15	0.63
1:D:184:ILE:HB	1:D:187:GLN:HB2	1.80	0.63
1:C:87:LEU:HD21	1:C:99:MET:HE3	1.81	0.63
1:A:6:LEU:HD11	1:A:239:GLU:HB3	1.82	0.62
1:D:166:TRP:HB2	1:D:229:GLU:HG3	1.79	0.62
1:C:173:LEU:HA	1:C:179:LEU:HD23	1.81	0.62
1:A:101:ARG:NH2	1:A:335:GLN:OE1	2.32	0.61
1:D:312:GLY:N	1:D:316:GLU:OE2	2.34	0.59
1:B:101:ARG:NH2	1:B:335:GLN:OE1	2.34	0.59
1:A:397:VAL:HG11	1:A:401:ILE:HD11	1.85	0.59
1:C:109:ILE:HB	1:C:234:GLY:HA3	1.83	0.58
1:D:168:VAL:HG21	1:D:322:TRP:CH2	2.38	0.58
1:C:81:LEU:HD22	1:C:320:THR:HB	1.84	0.58
1:C:142:GLN:N	1:C:142:GLN:OE1	2.37	0.58
1:D:151:TYR:HE1	1:D:317:GLU:HG2	1.69	0.58
1:D:68:ALA:HB3	1:D:317:GLU:HG3	1.84	0.58
1:D:273:GLU:HB3	1:D:290:GLN:HG3	1.86	0.58
1:C:246:THR:HB	1:C:262:GLU:CD	2.28	0.57
1:D:101:ARG:NE	1:D:332:ASP:OD1	2.37	0.56
1:A:316:GLU:HG2	1:A:317:GLU:N	2.20	0.56
1:C:424:PHE:HE2	1:C:454:ASN:HB2	1.70	0.56
1:A:87:LEU:HD21	1:A:99:MET:HG3	1.87	0.56
1:A:82:ALA:HB1	1:A:87:LEU:HB2	1.88	0.56
1:A:100:LEU:O	1:A:104:MET:HG3	2.06	0.55
1:D:82:ALA:HB1	1:D:87:LEU:HB2	1.88	0.55
1:D:6:LEU:O	1:D:256:ASN:ND2	2.36	0.55
1:D:233:VAL:HG11	1:D:241:VAL:HB	1.89	0.54
1:D:140:HIS:NE2	1:D:311:ALA:O	2.31	0.54
1:C:141:GLU:HB3	1:D:475:ALA:O	2.08	0.54
1:D:151:TYR:CE1	1:D:317:GLU:HG2	2.43	0.54
1:A:151:TYR:HE1	1:A:317:GLU:HG2	1.73	0.54
1:A:402:ASP:OD1	1:A:404:THR:HB	2.09	0.53
1:B:288:LYS:HE3	1:B:290:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD22	1:A:310:VAL:HG22	1.90	0.53
1:A:151:TYR:CE1	1:A:317:GLU:HG2	2.43	0.53
1:D:52:HIS:HA	1:D:62:ARG:HG2	1.90	0.53
1:D:224:PRO:HG2	1:D:227:VAL:HG21	1.90	0.53
1:A:68:ALA:HB3	1:A:317:GLU:HG3	1.89	0.52
1:A:46:ALA:HB2	1:B:496:ALA:HB1	1.91	0.52
1:B:190:GLY:O	1:B:194:GLU:HG2	2.09	0.52
1:B:345:TRP:CD1	1:B:404:THR:HA	2.45	0.52
1:D:320:THR:O	1:D:324:THR:OG1	2.22	0.51
1:B:233:VAL:HG11	1:B:241:VAL:HB	1.92	0.51
1:C:191:ILE:O	1:C:194:GLU:HG2	2.11	0.51
1:B:478:THR:O	1:B:482:ARG:HG2	2.10	0.51
1:B:382:VAL:HG11	1:B:394:LEU:HD21	1.93	0.51
1:A:457:TYR:HB2	1:A:460:GLN:HG3	1.92	0.51
1:C:68:ALA:HB3	1:C:317:GLU:HG3	1.93	0.50
1:C:127:GLU:OE1	1:C:176:ARG:NH2	2.45	0.50
1:C:316:GLU:HG2	1:C:317:GLU:N	2.26	0.50
1:C:87:LEU:HD11	1:C:99:MET:HG2	1.94	0.50
1:C:114:LEU:HD22	1:C:242:GLU:HB3	1.93	0.50
1:A:263:GLY:HA3	1:A:294:HIS:O	2.11	0.50
1:A:329:GLN:O	1:A:333:VAL:HG23	2.11	0.50
1:D:131:LEU:HD13	1:D:179:LEU:HD21	1.93	0.50
1:D:345:TRP:CD1	1:D:404:THR:HA	2.47	0.50
1:D:84:HIS:NE2	3:D:628:HOH:O	2.35	0.49
1:C:197:ARG:HG3	1:C:267:LEU:HD22	1.93	0.49
1:B:329:GLN:O	1:B:333:VAL:HG23	2.13	0.49
1:B:82:ALA:HB1	1:B:87:LEU:HB2	1.95	0.49
1:C:93:PRO:HB3	1:C:345:TRP:CZ3	2.48	0.48
1:A:130:ASP:OD1	1:A:132:THR:OG1	2.30	0.48
1:C:473:ARG:HA	1:C:481:ARG:HD3	1.96	0.48
1:C:263:GLY:HA3	1:C:294:HIS:O	2.14	0.48
1:C:241:VAL:HG12	3:C:509:HOH:O	2.13	0.48
1:A:280:HIS:CD2	1:A:282:TYR:H	2.23	0.48
1:B:87:LEU:HD21	1:B:99:MET:HG2	1.96	0.48
1:B:130:ASP:OD1	1:B:132:THR:OG1	2.30	0.47
1:A:22:VAL:HG23	1:A:47:PRO:HB2	1.96	0.47
1:B:361:VAL:HG11	1:B:460:GLN:NE2	2.29	0.47
1:C:280:HIS:HB2	1:C:436:PRO:HG3	1.97	0.47
1:D:30:ALA:HA	1:D:34:ILE:HD12	1.96	0.47
1:D:16:ARG:HD3	1:D:23:ASP:OD2	2.14	0.47
1:D:101:ARG:NH2	1:D:335:GLN:OE1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ASP:CG	1:B:363:ARG:HD3	2.40	0.47
1:B:58:LEU:HD12	1:B:59:PRO:HD2	1.96	0.46
1:B:183:THR:HG21	1:B:193:ARG:CD	2.45	0.46
1:A:16:ARG:HA	1:A:21:LEU:HB3	1.97	0.46
1:C:41:VAL:HG22	1:C:46:ALA:HB3	1.97	0.46
1:B:102:ALA:O	1:B:105:ARG:HG2	2.14	0.46
1:B:119:VAL:HG21	1:B:260:VAL:HG23	1.96	0.46
1:D:222:PRO:HD3	1:D:329:GLN:NE2	2.30	0.46
1:B:168:VAL:HG21	1:B:322:TRP:HZ2	1.81	0.46
1:B:14:HIS:O	1:B:18:GLN:HG2	2.16	0.46
1:A:101:ARG:HD2	1:A:331:LEU:HD23	1.98	0.46
1:B:73:ASP:OD2	1:B:76:ARG:HD2	2.15	0.46
1:A:389:HIS:O	1:A:432:PHE:HB2	2.16	0.46
1:B:316:GLU:OE1	1:B:318:ASN:HB2	2.16	0.46
1:A:87:LEU:HD11	1:A:99:MET:HG3	1.98	0.45
1:A:119:VAL:HG21	1:A:260:VAL:HG23	1.98	0.45
1:B:71:ARG:HD3	1:B:76:ARG:O	2.16	0.45
1:A:173:LEU:HA	1:A:179:LEU:HD23	1.98	0.45
1:C:147:TYR:CE2	1:C:172:MET:HB2	2.52	0.45
1:D:170:ARG:NH1	1:D:276:MET:HB3	2.32	0.45
1:B:87:LEU:HD11	1:B:99:MET:HG2	1.98	0.45
1:B:483:ARG:O	1:B:487:ARG:HB2	2.16	0.45
1:A:325:MET:O	1:A:329:GLN:HG3	2.17	0.45
1:B:20:ASP:OD1	1:B:80:ARG:NH2	2.41	0.45
1:C:271:ALA:HB2	1:C:292:LEU:HD21	1.97	0.45
1:D:315:PRO:HG2	3:D:644:HOH:O	2.15	0.45
1:B:311:ALA:HA	1:B:316:GLU:HG3	1.98	0.45
1:D:256:ASN:O	1:D:301:ARG:HD2	2.16	0.45
1:B:4:SER:OG	1:B:14:HIS:ND1	2.42	0.45
1:D:316:GLU:HG3	1:D:318:ASN:H	1.81	0.45
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.78	0.45
1:A:183:THR:HG21	1:A:193:ARG:CD	2.47	0.45
1:A:96:ILE:O	1:A:100:LEU:HG	2.17	0.44
1:A:1:MET:HE3	1:A:88:PRO:HA	2.00	0.44
1:B:147:TYR:OH	1:B:273:GLU:OE2	2.24	0.44
1:B:265:ILE:HG12	1:B:293:PHE:CE2	2.52	0.44
1:B:316:GLU:HG2	1:B:317:GLU:N	2.32	0.44
1:C:14:HIS:ND1	1:C:83:LEU:HD11	2.32	0.44
1:C:234:GLY:HA2	1:C:239:GLU:O	2.17	0.44
1:B:118:PRO:HD2	1:B:255:ALA:O	2.18	0.44
1:C:14:HIS:O	1:C:18:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:HIS:HA	1:C:191:ILE:HD12	2.00	0.44
1:C:316:GLU:OE2	1:C:318:ASN:HB2	2.18	0.44
1:B:163:TRP:CD2	1:B:226:GLY:HA2	2.53	0.44
1:D:432:PHE:CE2	1:D:434:MET:HB2	2.52	0.44
1:B:76:ARG:HG2	1:B:89:GLU:HG2	1.99	0.44
1:C:80:ARG:NH2	3:C:504:HOH:O	2.43	0.43
1:D:246:THR:HB	1:D:262:GLU:CD	2.43	0.43
1:D:340:PRO:HD3	1:D:367:LEU:HD11	2.00	0.43
1:D:273:GLU:HB3	1:D:290:GLN:CG	2.49	0.43
1:A:147:TYR:OH	1:A:273:GLU:OE2	2.24	0.43
1:B:488:TRP:HA	1:B:491:TYR:HD2	1.83	0.43
1:D:361:VAL:HA	1:D:364:LEU:HB3	2.00	0.43
1:A:485:GLU:HG2	1:B:40:ARG:CZ	2.48	0.43
1:A:52:HIS:HA	1:A:62:ARG:HG2	2.01	0.43
1:B:109:ILE:HG22	1:B:240:PRO:HB3	2.01	0.43
1:D:263:GLY:HA3	1:D:294:HIS:O	2.18	0.43
1:D:223:LEU:HA	1:D:224:PRO:HD2	1.78	0.43
1:D:223:LEU:HD13	1:D:227:VAL:HG12	2.01	0.43
1:A:234:GLY:HA2	1:A:239:GLU:O	2.19	0.43
1:C:101:ARG:NH2	1:C:335:GLN:OE1	2.52	0.43
1:C:193:ARG:HD2	1:C:265:ILE:HG21	2.00	0.43
1:D:5:ALA:HB1	1:D:214:ALA:HB2	2.00	0.43
1:C:140:HIS:HB2	1:C:143:ASP:OD1	2.18	0.43
1:C:345:TRP:CD1	1:C:404:THR:HA	2.54	0.43
1:D:321:ILE:O	1:D:325:MET:HG3	2.19	0.43
1:B:432:PHE:CD1	1:B:433:PRO:HD2	2.54	0.42
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.82	0.42
1:D:361:VAL:HG11	1:D:460:GLN:NE2	2.34	0.42
1:A:122:ASN:O	1:A:299:SER:HA	2.19	0.42
1:A:140:HIS:NE2	1:A:311:ALA:O	2.50	0.42
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.94	0.42
1:D:478:THR:O	1:D:482:ARG:HG2	2.19	0.42
1:C:180:ALA:O	1:C:273:GLU:HG3	2.19	0.42
1:C:476:TYR:HA	1:C:477:PRO:HD3	1.91	0.42
1:B:183:THR:HG21	1:B:193:ARG:HD3	2.02	0.42
1:C:158:THR:HG22	1:C:163:TRP:O	2.20	0.42
1:C:183:THR:HG21	1:C:193:ARG:CD	2.47	0.42
1:B:263:GLY:HA3	1:B:294:HIS:O	2.20	0.42
1:C:163:TRP:CG	1:C:226:GLY:HA2	2.55	0.42
1:D:32:LEU:HD23	1:D:32:LEU:HA	1.90	0.42
1:A:154:HIS:CE1	1:A:207:MET:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLN:HB3	1:C:251:LEU:CD2	2.49	0.42
1:B:168:VAL:HG21	1:B:322:TRP:CZ2	2.55	0.41
1:D:413:LEU:HD12	1:D:413:LEU:HA	1.92	0.41
1:A:360:ASP:OD2	1:A:363:ARG:HD3	2.20	0.41
1:A:402:ASP:C	1:A:404:THR:H	2.28	0.41
1:A:473:ARG:HA	1:A:481:ARG:HD3	2.02	0.41
1:C:221:MET:HB2	1:C:325:MET:HE1	2.02	0.41
1:B:103:ALA:HB1	1:B:236:LEU:HD12	2.02	0.41
1:B:364:LEU:HD11	1:B:461:PHE:CE2	2.55	0.41
1:D:143:ASP:OD1	1:D:276:MET:HA	2.21	0.41
1:C:206:ALA:HA	1:C:261:LEU:O	2.20	0.41
1:D:49:PRO:HD2	1:D:65:GLY:O	2.21	0.41
1:D:382:VAL:O	1:D:388:GLY:HA3	2.19	0.41
1:B:317:GLU:HA	1:B:320:THR:OG1	2.20	0.41
1:C:330:LEU:HD23	1:C:330:LEU:HA	1.86	0.41
1:C:389:HIS:O	1:C:432:PHE:HB2	2.20	0.41
1:D:168:VAL:HG21	1:D:322:TRP:CZ2	2.54	0.41
1:A:432:PHE:HA	1:A:433:PRO:HD3	1.83	0.41
1:C:321:ILE:O	1:C:325:MET:HG3	2.20	0.41
1:A:393:LYS:HE3	1:A:437:TYR:CE2	2.56	0.41
1:B:156:VAL:HG12	1:B:204:PRO:O	2.21	0.41
1:B:354:TRP:C	1:B:354:TRP:CD1	2.99	0.41
1:A:273:GLU:HB3	1:A:290:GLN:HG3	2.03	0.41
1:B:23:ASP:OD1	1:B:52:HIS:NE2	2.41	0.41
1:B:340:PRO:HD3	1:B:367:LEU:HD11	2.03	0.41
1:B:434:MET:HE2	1:B:434:MET:HB3	1.96	0.41
1:C:271:ALA:O	1:C:289:PRO:HA	2.21	0.41
1:D:16:ARG:NH1	1:D:23:ASP:OD1	2.53	0.41
1:C:155:VAL:HB	1:C:206:ALA:HB3	2.03	0.41
1:A:393:LYS:HE3	1:A:437:TYR:CZ	2.56	0.40
1:C:163:TRP:CZ2	1:C:225:GLU:HG3	2.56	0.40
1:C:276:MET:HB3	1:C:276:MET:HE2	1.85	0.40
1:D:136:VAL:H	1:D:136:VAL:HG23	1.65	0.40
1:C:325:MET:HE2	1:C:325:MET:HB3	1.88	0.40
1:D:155:VAL:HG22	1:D:166:TRP:CD1	2.56	0.40
1:A:87:LEU:HA	1:A:88:PRO:HD2	1.74	0.40
1:A:156:VAL:HG23	1:A:192:ILE:HD12	2.03	0.40
1:B:383:PHE:CD2	1:B:450:ARG:HD2	2.56	0.40
1:A:66:ALA:N	1:A:67:PRO:HD3	2.36	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	491/518 (95%)	472 (96%)	19 (4%)	0	100	100
1	B	493/518 (95%)	478 (97%)	14 (3%)	1 (0%)	43	55
1	C	487/518 (94%)	471 (97%)	16 (3%)	0	100	100
1	D	491/518 (95%)	469 (96%)	21 (4%)	1 (0%)	43	55
All	All	1962/2072 (95%)	1890 (96%)	70 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	219	ALA
1	D	32	LEU

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	392/413 (95%)	383 (98%)	9 (2%)	44	63
1	B	392/413 (95%)	379 (97%)	13 (3%)	33	50
1	C	390/413 (94%)	378 (97%)	12 (3%)	35	52
1	D	392/413 (95%)	382 (97%)	10 (3%)	40	59
All	All	1566/1652 (95%)	1522 (97%)	44 (3%)	38	56

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	SER
1	A	186	THR
1	A	216	LEU
1	A	280	HIS
1	A	286	ILE
1	A	316	GLU
1	A	352	THR
1	A	354	TRP
1	A	404	THR
1	B	3	ARG
1	B	81	LEU
1	B	158	THR
1	B	178	THR
1	B	199	LEU
1	B	303	GLN
1	B	316	GLU
1	B	332	ASP
1	B	336	ASN
1	B	347	SER
1	B	352	THR
1	B	354	TRP
1	B	361	VAL
1	C	39	ARG
1	C	83	LEU
1	C	114	LEU
1	C	141	GLU
1	C	157	GLN
1	C	167	SER
1	C	168	VAL
1	C	178	THR
1	C	286	ILE
1	C	316	GLU
1	C	352	THR
1	C	401	ILE
1	D	2	ASN
1	D	16	ARG
1	D	39	ARG
1	D	80	ARG
1	D	127	GLU
1	D	136	VAL
1	D	229	GLU
1	D	267	LEU
1	D	347	SER

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Mol	Chain	Res	Type
1	D	354	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	14	HIS
1	A	18	GLN
1	A	78	HIS
1	A	157	GLN
1	A	188	HIS
1	A	280	HIS
1	B	389	HIS
1	B	474	HIS
1	C	187	GLN
1	C	318	ASN
1	C	464	GLN
1	D	31	ASN
1	D	78	HIS
1	D	247	GLN
1	D	474	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.22	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	493/518 (95%)	-1.55	0 100 100	9, 22, 41, 57	3 (0%)
1	B	495/518 (95%)	-1.53	0 100 100	9, 23, 44, 72	3 (0%)
1	C	491/518 (94%)	-1.46	0 100 100	12, 26, 47, 81	8 (1%)
1	D	493/518 (95%)	-1.52	0 100 100	12, 24, 44, 64	8 (1%)
All	All	1972/2072 (95%)	-1.52	0 100 100	9, 24, 44, 81	22 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	SO4	D	501	5/5	0.99	0.05	52,64,66,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.