Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 09:40 AM JST

PDB ID	:	8WVR
Title	:	Complex structure of the azoxy synthase VlmB and its substrate
Authors	:	Zang, X.; Zhou, J.H.; Yiling, D.; Jingkun, S.; Zhijie, Z.; Zhuanglin, S.; Guiyun, Z.
Deposited on	:	2023-10-24
Resolution	:	2.05 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:

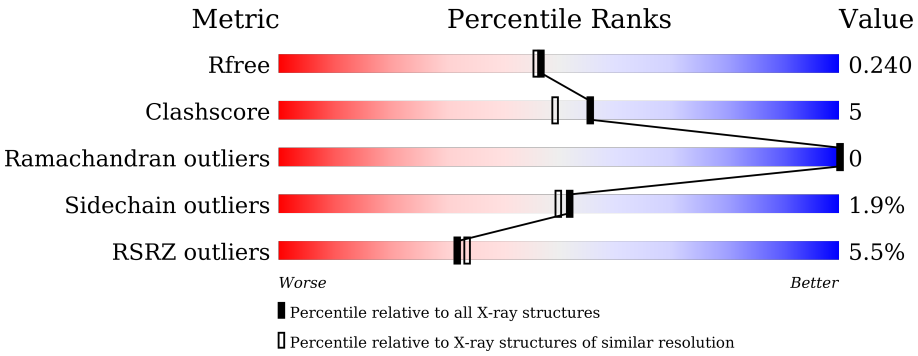
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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 <=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	332	89% 7%
1	B	332	3% 88% 9%
1	C	332	4% 84% 11%
1	D	332	14% 82% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10691 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 Putative VlmB homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2516	1578	461	467	10			
1	B	323	Total	C	N	O	S	0	0	0
			2516	1578	461	467	10			
1	C	318	Total	C	N	O	S	0	0	0
			2474	1552	453	459	10			
1	D	322	Total	C	N	O	S	0	0	0
			2508	1574	460	464	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	HIS	-	expression tag	UNP E4N6B3
A	328	HIS	-	expression tag	UNP E4N6B3
A	329	HIS	-	expression tag	UNP E4N6B3
A	330	HIS	-	expression tag	UNP E4N6B3
A	331	HIS	-	expression tag	UNP E4N6B3
A	332	HIS	-	expression tag	UNP E4N6B3
B	327	HIS	-	expression tag	UNP E4N6B3
B	328	HIS	-	expression tag	UNP E4N6B3
B	329	HIS	-	expression tag	UNP E4N6B3
B	330	HIS	-	expression tag	UNP E4N6B3
B	331	HIS	-	expression tag	UNP E4N6B3
B	332	HIS	-	expression tag	UNP E4N6B3
C	327	HIS	-	expression tag	UNP E4N6B3
C	328	HIS	-	expression tag	UNP E4N6B3
C	329	HIS	-	expression tag	UNP E4N6B3
C	330	HIS	-	expression tag	UNP E4N6B3
C	331	HIS	-	expression tag	UNP E4N6B3
C	332	HIS	-	expression tag	UNP E4N6B3
D	327	HIS	-	expression tag	UNP E4N6B3
D	328	HIS	-	expression tag	UNP E4N6B3
D	329	HIS	-	expression tag	UNP E4N6B3

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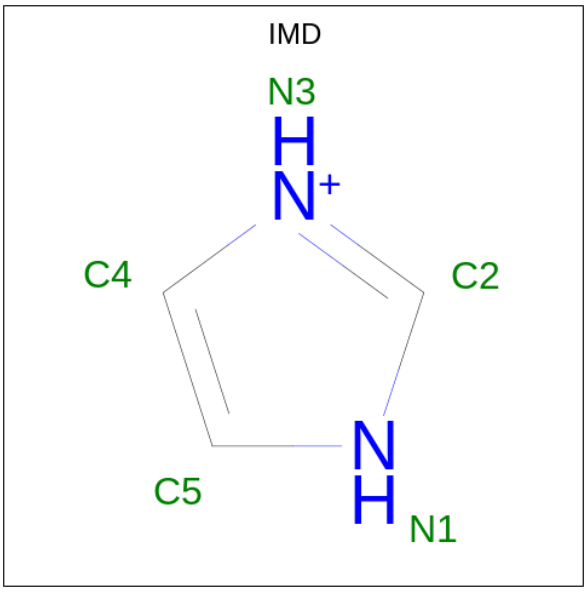
Chain	Residue	Modelled	Actual	Comment	Reference
D	330	HIS	-	expression tag	UNP E4N6B3
D	331	HIS	-	expression tag	UNP E4N6B3
D	332	HIS	-	expression tag	UNP E4N6B3

- Molecule 2 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).

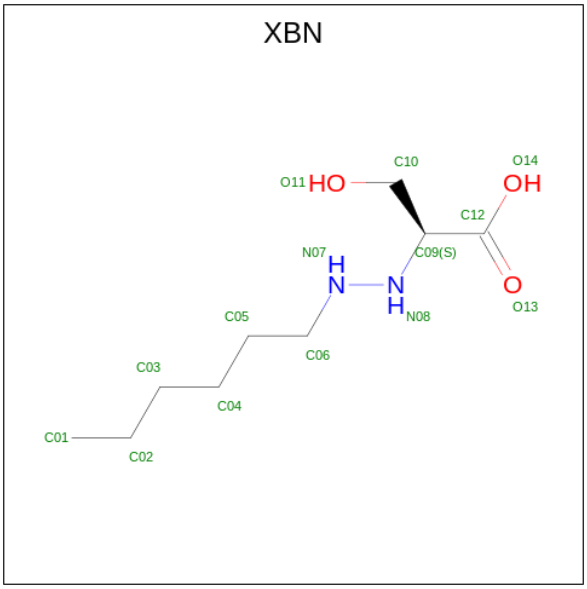


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 5 3 2	0	0
2	B	1	Total C N 5 3 2	0	0
2	C	1	Total C N 5 3 2	0	0
2	D	1	Total C N 5 3 2	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Fe 2 2	0	0
3	B	2	Total Fe 2 2	0	0
3	C	2	Total Fe 2 2	0	0
3	D	2	Total Fe 2 2	0	0

- Molecule 4 is (2 {S})-2-(2-hexylhydrazinyl)-3-oxidanyl-propanoic acid (three-letter code: XBN) (formula: $C_9H_{20}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N O 14 9 2 3	0	0

- Molecule 5 is water.

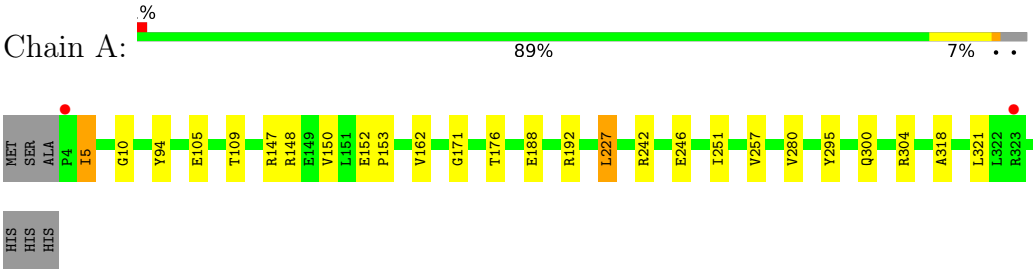
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	208	Total O 208 208	0	0
5	B	177	Total O 177 177	0	0
5	C	188	Total O 188 188	0	0
5	D	62	Total O 62 62	0	0

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.

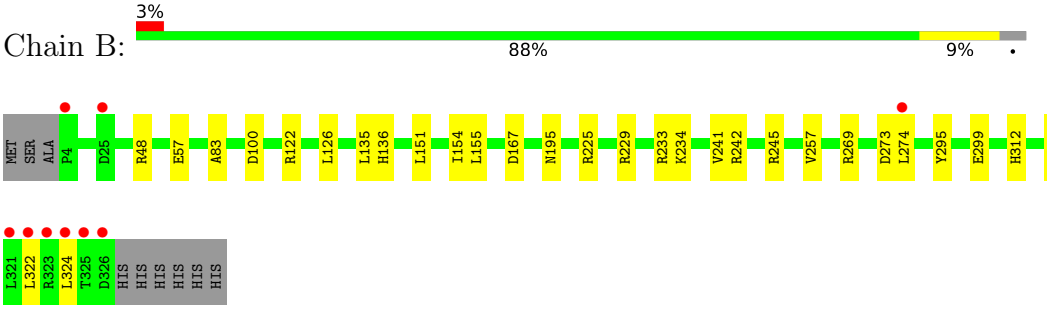
• Molecule 1: Putative VlmB homolog

Chain A:



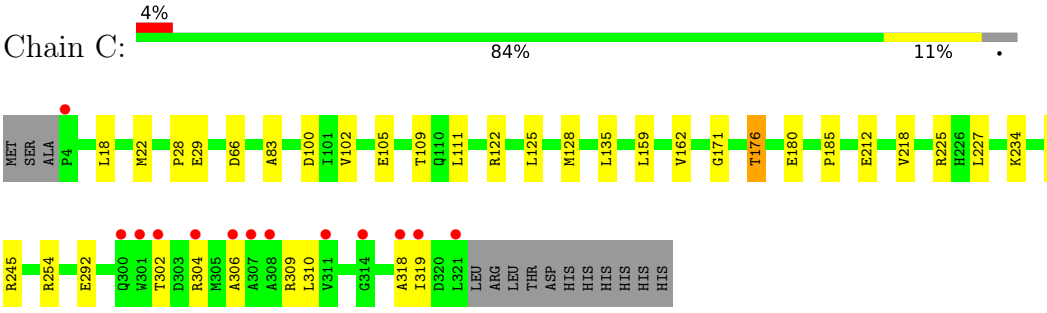
• Molecule 1: Putative VlmB homolog

Chain B:



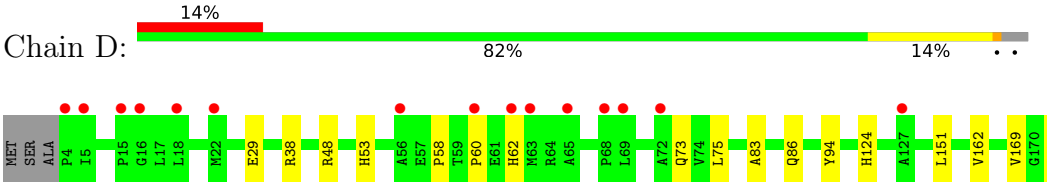
• Molecule 1: Putative VlmB homolog

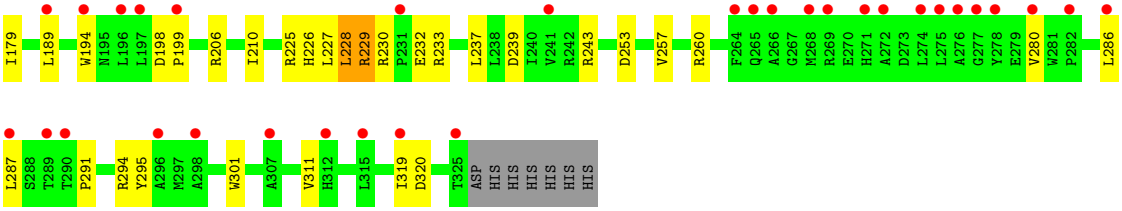
Chain C:



• Molecule 1: Putative VlmB homolog

Chain D:




I179
L189
W194
N195
L196
L197
D198
P199
R206
I210
R225
H226
L227
L228
R229
R230
P231
E232
R233
L237
L238
D239
I240
V241
R242
R243
D253
V257
R260
F264
Q265
A266
G267
M268
R269
E270
H271
A272
D273
L274
L275
A276
G277
Y278
E279
V280
W281
P282
L286
L287
S288
T289
T290
P291
R294
Y295
A296
M297
A298
W301
A307
V311
H312
L315
I319
D320
T325
ASP
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.82Å 95.18Å 183.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.88 – 2.05 33.88 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.88-2.05) 100.0 (33.88-2.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.195 , 0.240 0.195 , 0.240	Depositor DCC
R_{free} test set	4829 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10691	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XBN, IMD, FE

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	0/2568	0.61	0/3492
1	B	0.39	0/2568	0.63	0/3492
1	C	0.40	0/2526	0.62	0/3435
1	D	0.30	0/2560	0.56	0/3481
All	All	0.38	0/10222	0.60	0/13900

There are no bond length outliers.

There are no bond angle outliers.

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	2516	0	2500	16	0
1	B	2516	0	2500	20	0
1	C	2474	0	2454	29	0
1	D	2508	0	2496	29	0
2	A	5	0	4	0	0
2	B	5	0	4	0	0
2	C	5	0	4	0	0
2	D	5	0	5	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	C	14	0	0	3	0
5	A	208	0	0	1	1
5	B	177	0	0	4	0
5	C	188	0	0	6	1
5	D	62	0	0	4	0
All	All	10691	0	9967	92	1

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 5.

All (92) 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:245:ARG:NH1	5:C:501:HOH:O	2.15	0.79
1:B:225:ARG:HG2	1:B:225:ARG:HH11	1.55	0.72
1:C:18:LEU:O	1:C:22:MET:HG3	1.91	0.69
1:B:122:ARG:HG2	1:B:135:LEU:HD21	1.74	0.68
1:B:320:ASP:OD2	5:B:501:HOH:O	2.12	0.66
1:B:312:HIS:HB2	1:C:304:ARG:HD3	1.78	0.66
1:D:243:ARG:NH2	5:D:502:HOH:O	2.29	0.66
1:C:162:VAL:CG2	1:C:171:GLY:HA3	2.30	0.62
1:A:300:GLN:OE1	1:A:304:ARG:NH1	2.33	0.62
1:C:162:VAL:HG23	1:C:171:GLY:HA3	1.81	0.62
1:A:162:VAL:HG22	1:A:171:GLY:HA3	1.82	0.61
1:D:83:ALA:HA	1:D:151:LEU:HD21	1.82	0.61
1:B:229:ARG:NH1	5:B:505:HOH:O	2.31	0.61
1:C:176:THR:HG23	5:C:505:HOH:O	2.01	0.60
1:B:83:ALA:HA	1:B:151:LEU:HD21	1.83	0.60
1:C:66:ASP:OD1	5:C:502:HOH:O	2.17	0.60
1:A:162:VAL:CG2	1:A:171:GLY:HA3	2.33	0.58
1:B:245:ARG:HB2	1:B:322:LEU:HD23	1.86	0.58
1:D:75:LEU:HD23	1:D:260:ARG:HB3	1.85	0.58
1:D:257:VAL:HG21	1:D:295:TYR:CE1	2.41	0.56
1:C:100:ASP:OD2	5:C:503:HOH:O	2.18	0.56
1:B:299:GLU:OE2	1:B:324:LEU:HB3	2.06	0.55
1:A:94:TYR:CZ	1:A:162:VAL:HG21	2.43	0.52
1:A:148:ARG:NH1	5:A:509:HOH:O	2.42	0.52
1:B:241:VAL:HG11	1:B:318:ALA:HB1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ARG:HB3	5:D:511:HOH:O	2.08	0.52
1:D:232:GLU:O	5:D:501:HOH:O	2.19	0.51
1:C:302:THR:O	1:C:306:ALA:N	2.29	0.51
1:D:227:LEU:HD21	1:D:237:LEU:HD12	1.94	0.50
1:C:83:ALA:HB1	4:C:402:XBN:C02	2.43	0.49
1:B:234:LYS:HE2	1:B:317:GLU:OE2	2.13	0.49
1:C:176:THR:HG22	1:C:309:ARG:HH12	1.77	0.49
1:C:242:ARG:HD3	5:C:661:HOH:O	2.12	0.49
1:D:311:VAL:HG13	1:D:319:ILE:HD11	1.95	0.48
1:B:245:ARG:HB2	1:B:322:LEU:CD2	2.43	0.48
1:B:269:ARG:O	5:B:502:HOH:O	2.20	0.48
1:C:254:ARG:NH2	1:C:292:GLU:OE2	2.46	0.48
1:A:257:VAL:HG11	1:A:295:TYR:HD1	1.78	0.48
1:D:58:PRO:HD2	1:D:199:PRO:HB2	1.95	0.47
1:C:310:LEU:HD13	1:C:318:ALA:HB3	1.95	0.47
1:A:192:ARG:HD3	1:A:280:VAL:O	2.14	0.47
1:B:136:HIS:HD2	5:B:664:HOH:O	1.95	0.47
1:B:274:LEU:HD12	1:B:274:LEU:H	1.79	0.47
1:A:153:PRO:HB2	1:A:251:ILE:HD11	1.97	0.46
1:C:125:LEU:HD23	1:C:128:MET:CE	2.46	0.46
1:D:86:GLN:NE2	5:D:504:HOH:O	2.48	0.46
1:D:29:GLU:OE2	1:D:225:ARG:NH1	2.49	0.45
1:D:124:HIS:HE1	1:D:198:ASP:OD2	1.99	0.45
1:D:60:PRO:HB2	1:D:62:HIS:CD2	2.50	0.45
1:B:312:HIS:HB2	1:C:304:ARG:CD	2.47	0.45
1:B:257:VAL:HG11	1:B:295:TYR:HD1	1.82	0.45
1:C:238:LEU:O	1:C:242:ARG:HG3	2.17	0.45
1:A:150:VAL:HG22	1:A:251:ILE:HG23	1.98	0.45
1:A:318:ALA:HA	1:A:321:LEU:HD12	1.98	0.45
1:A:242:ARG:NH1	1:A:246:GLU:OE2	2.48	0.45
1:C:238:LEU:HD23	1:C:238:LEU:HA	1.84	0.44
1:A:147:ARG:HD2	1:A:152:GLU:OE2	2.18	0.44
1:C:125:LEU:HD23	1:C:128:MET:HE3	2.00	0.44
1:A:5:ILE:HD11	1:A:10:GLY:HA2	2.00	0.43
1:B:126:LEU:HD21	1:B:135:LEU:HD22	2.00	0.43
1:B:154:ILE:HG13	1:B:155:LEU:N	2.33	0.43
1:D:189:LEU:HD21	1:D:294:ARG:HB3	2.00	0.43
1:D:253:ASP:O	1:D:257:VAL:HG22	2.18	0.43
1:D:73:GLN:HB2	1:D:194:TRP:CH2	2.54	0.43
1:C:28:PRO:HD3	1:C:218:VAL:HG13	2.00	0.43
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:VAL:HB	1:D:286:LEU:HD13	2.01	0.43
1:D:38:ARG:HA	1:D:38:ARG:HD2	1.90	0.42
1:C:122:ARG:HG2	1:C:135:LEU:HD21	2.00	0.42
1:C:180:GLU:OE2	4:C:402:XBN:N07	2.53	0.42
1:D:60:PRO:HD3	1:D:199:PRO:HD2	2.00	0.42
1:C:234:LYS:NZ	5:C:517:HOH:O	2.52	0.42
1:D:228:LEU:O	1:D:230:ARG:HG2	2.19	0.42
1:A:257:VAL:HG11	1:A:295:TYR:CD1	2.55	0.42
1:D:162:VAL:HG22	1:D:171:GLY:HA3	2.02	0.42
1:D:169:VAL:HG11	1:D:226:HIS:CG	2.55	0.42
1:D:226:HIS:CE1	1:D:233:ARG:HD3	2.55	0.42
1:C:185:PRO:HG2	1:C:302:THR:OG1	2.20	0.42
1:D:94:TYR:CZ	1:D:162:VAL:HG21	2.55	0.41
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.84	0.41
1:D:189:LEU:HB2	1:D:301:TRP:HZ3	1.84	0.41
1:B:48:ARG:HH12	1:B:57:GLU:CD	2.24	0.41
1:B:167:ASP:OD1	1:B:233:ARG:NH2	2.51	0.41
1:C:29:GLU:HG3	1:C:102:VAL:HG11	2.01	0.41
1:D:206:ARG:O	1:D:210:ILE:HG13	2.20	0.41
1:A:105:GLU:O	1:A:109:THR:HG23	2.20	0.41
1:D:175:PHE:HA	1:D:179:ILE:HD12	2.03	0.41
1:C:105:GLU:O	1:C:109:THR:HG23	2.20	0.41
1:C:122:ARG:CG	1:C:135:LEU:HD21	2.52	0.40
1:C:212:GLU:OE2	4:C:402:XBN:O11	2.39	0.40
1:D:48:ARG:HH11	1:D:53:HIS:HA	1.86	0.40
1:D:291:PRO:HA	1:D:294:ARG:HH21	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:674:HOH:O	5:C:591:HOH:O[4_545]	2.17	0.03

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	321/332 (97%)	315 (98%)	6 (2%)	0	100	100
1	B	321/332 (97%)	315 (98%)	6 (2%)	0	100	100
1	C	316/332 (95%)	309 (98%)	7 (2%)	0	100	100
1	D	320/332 (96%)	309 (97%)	11 (3%)	0	100	100
All	All	1278/1328 (96%)	1248 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	257/265 (97%)	253 (98%)	4 (2%)	58	57
1	B	257/265 (97%)	252 (98%)	5 (2%)	52	50
1	C	252/265 (95%)	247 (98%)	5 (2%)	50	47
1	D	256/265 (97%)	251 (98%)	5 (2%)	50	47
All	All	1022/1060 (96%)	1003 (98%)	19 (2%)	52	50

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	176	THR
1	A	188	GLU
1	A	227	LEU
1	B	100	ASP
1	B	195	ASN
1	B	242	ARG
1	B	273	ASP
1	B	320	ASP
1	C	111	LEU

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Mol	Chain	Res	Type
1	C	159	LEU
1	C	176	THR
1	C	225	ARG
1	C	319	ILE
1	D	228	LEU
1	D	229	ARG
1	D	239	ASP
1	D	287	LEU
1	D	320	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 for Mogul analysis.

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	IMD	A	401	3	3,5,5	0.28	0	4,5,5	0.66	0
2	IMD	B	401	3	3,5,5	0.28	0	4,5,5	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	IMD	D	401	-	3,5,5	0.27	0	4,5,5	0.64	0
4	XBN	C	402	3	12,13,13	2.03	2 (16%)	11,14,14	1.50	3 (27%)
2	IMD	C	401	3	3,5,5	0.27	0	4,5,5	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	A	401	3	-	-	0/1/1/1
2	IMD	B	401	3	-	-	0/1/1/1
2	IMD	D	401	-	-	-	0/1/1/1
4	XBN	C	402	3	-	1/11/14/14	-
2	IMD	C	401	3	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	402	XBN	C06-N07	5.92	1.51	1.45
4	C	402	XBN	C09-C12	2.17	1.58	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	402	XBN	O11-C10-C09	-3.01	103.51	111.03
4	C	402	XBN	O14-C12-O13	-2.11	119.30	124.09
4	C	402	XBN	C10-C09-N08	2.07	114.42	108.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

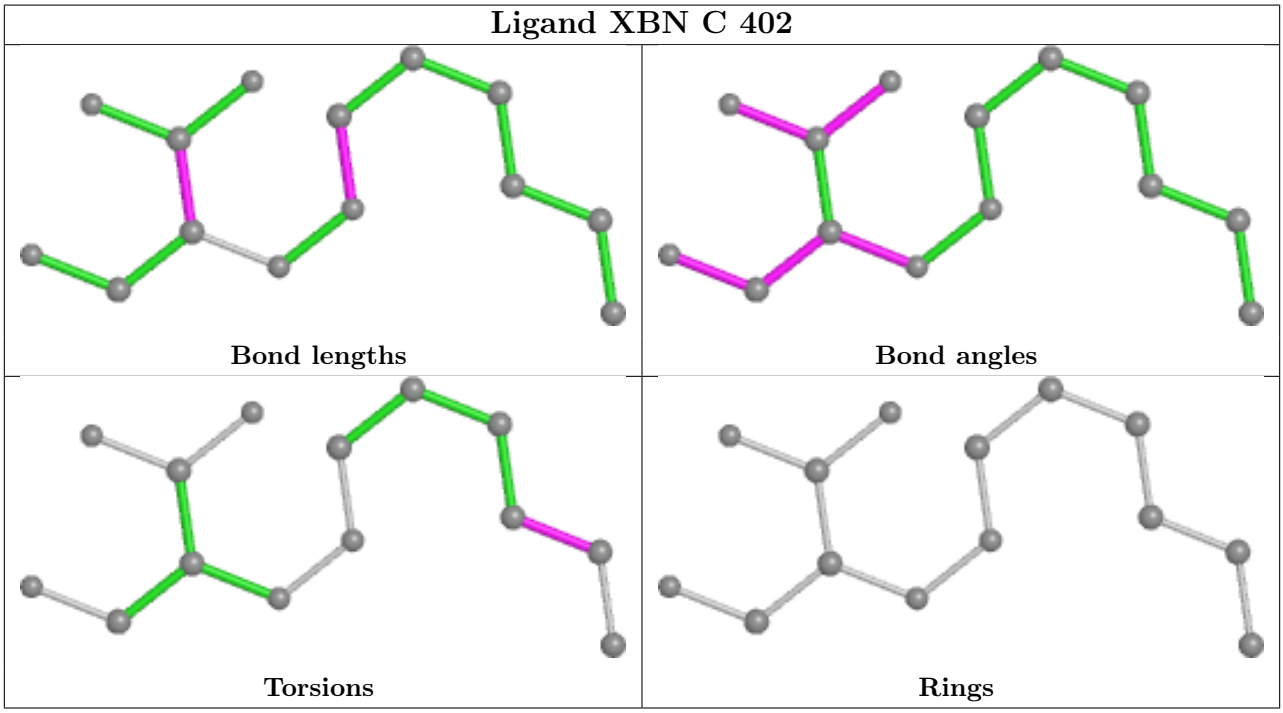
Mol	Chain	Res	Type	Atoms
4	C	402	XBN	C01-C02-C03-C04

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	402	XBN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/332 (97%)	-0.33	2 (0%) 85 88	21, 31, 42, 65	0
1	B	323/332 (97%)	-0.06	9 (2%) 55 57	21, 33, 49, 79	0
1	C	318/332 (95%)	-0.08	13 (4%) 42 44	21, 31, 49, 85	0
1	D	322/332 (96%)	1.03	47 (14%) 7 6	28, 54, 87, 97	0
All	All	1286/1328 (96%)	0.14	71 (5%) 32 33	21, 34, 70, 97	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	321	LEU	5.7
1	B	322	LEU	4.7
1	C	319	ILE	4.6
1	D	4	PRO	4.2
1	C	307	ALA	4.0
1	D	307	ALA	4.0
1	D	69	LEU	3.8
1	B	25	ASP	3.8
1	B	324	LEU	3.7
1	C	4	PRO	3.7
1	B	325	THR	3.7
1	D	264	PHE	3.6
1	C	306	ALA	3.6
1	D	287	LEU	3.5
1	D	276	ALA	3.5
1	D	231	PRO	3.5
1	C	311	VAL	3.4
1	D	274	LEU	3.3
1	D	275	LEU	3.2
1	B	323	ARG	3.2
1	B	4	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	18	LEU	3.1
1	B	274	LEU	3.1
1	D	282	PRO	3.0
1	D	72	ALA	3.0
1	D	269	ARG	3.0
1	D	68	PRO	2.9
1	D	63	MET	2.9
1	D	197	LEU	2.9
1	B	326	ASP	2.9
1	D	196	LEU	2.8
1	D	286	LEU	2.8
1	D	272	ALA	2.8
1	C	314	GLY	2.7
1	D	278	TYR	2.7
1	D	189	LEU	2.7
1	D	62	HIS	2.6
1	D	241	VAL	2.6
1	D	277	GLY	2.6
1	C	302	THR	2.6
1	D	271	HIS	2.6
1	C	318	ALA	2.6
1	D	56	ALA	2.6
1	D	199	PRO	2.6
1	D	325	THR	2.5
1	A	4	PRO	2.5
1	B	321	LEU	2.5
1	D	65	ALA	2.5
1	D	5	ILE	2.5
1	D	127	ALA	2.5
1	D	290	THR	2.4
1	D	60	PRO	2.4
1	C	304	ARG	2.4
1	D	289	THR	2.3
1	D	280	VAL	2.3
1	D	194	TRP	2.3
1	D	315	LEU	2.3
1	D	22	MET	2.3
1	D	312	HIS	2.2
1	D	266	ALA	2.2
1	C	300	GLN	2.2
1	D	296	ALA	2.2
1	D	319	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	308	ALA	2.1
1	D	298	ALA	2.1
1	D	16	GLY	2.1
1	C	301	TRP	2.1
1	D	265	GLN	2.0
1	D	15	PRO	2.0
1	A	323	ARG	2.0
1	D	268	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

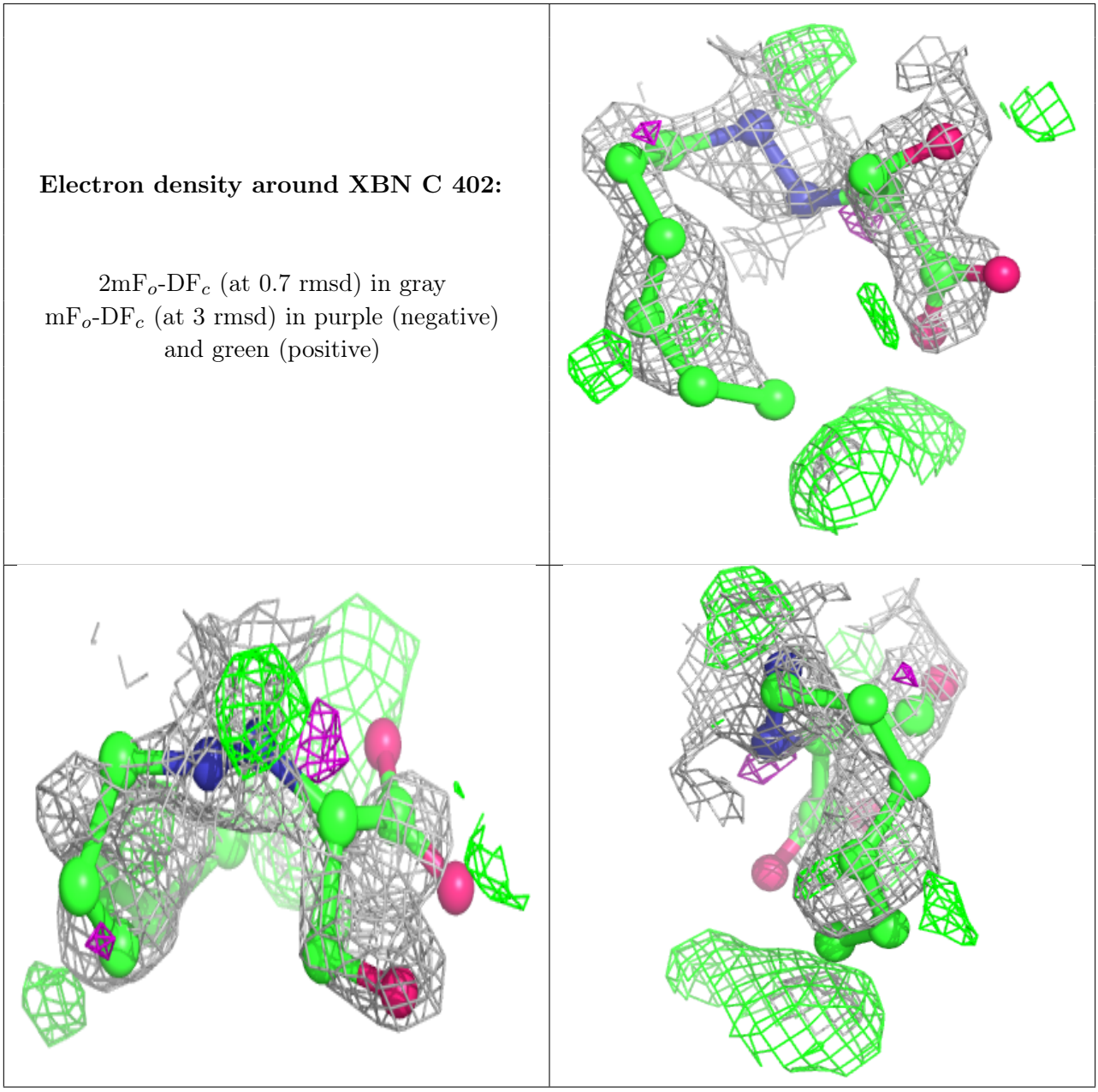
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	XBN	C	402	14/14	0.73	0.27	25,30,38,39	14
2	IMD	D	401	5/5	0.88	0.18	43,44,48,49	0
2	IMD	C	401	5/5	0.97	0.06	26,26,27,27	0
2	IMD	A	401	5/5	0.97	0.05	26,28,29,30	0
2	IMD	B	401	5/5	0.97	0.07	26,28,28,31	0
3	FE	A	403	1/1	0.99	0.03	25,25,25,25	0
3	FE	B	402	1/1	0.99	0.02	24,24,24,24	0
3	FE	C	404	1/1	0.99	0.02	23,23,23,23	0
3	FE	D	402	1/1	0.99	0.03	42,42,42,42	0
3	FE	D	403	1/1	0.99	0.04	39,39,39,39	0
3	FE	A	402	1/1	0.99	0.02	24,24,24,24	0
3	FE	B	403	1/1	1.00	0.01	24,24,24,24	0
3	FE	C	403	1/1	1.00	0.02	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around XBN C 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.