W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:53 PM GMT

PDB ID : 4WU3
Title : Structure of the PTP-like myo-inositol phosphatase from Mitsuokella multacida in complex with myo-inositol-(1,3,4,5)-tetrakisphosphate
Authors : Bruder, L.M.; Mosimann, S.C.
Deposited on : 2014-10-30
Resolution : 2.20 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:
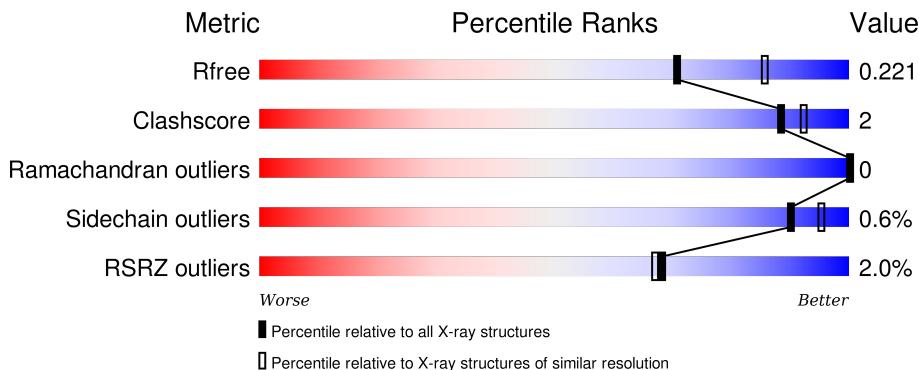
1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
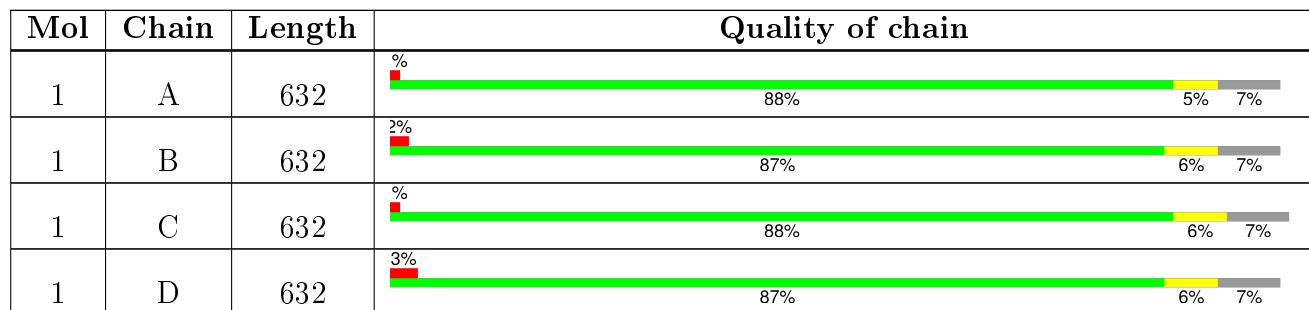
The reported resolution of this entry is 2.20 Å.

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	Percentile Ranks	Value
Rfree		0.221
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		2.0%

Worse *Better*

▮ Percentile relative to all X-ray structures
⬚ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 <=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	632	% 88% 5% 7%
1	B	632	2% 87% 6% 7%
1	C	632	% 88% 6% 7%
1	D	632	3% 87% 6% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	4IP	A	701	-	-	-	X
2	4IP	A	702	-	-	-	X
2	4IP	B	701	-	-	-	X
2	4IP	C	701	-	-	-	X
2	4IP	C	702	-	-	-	X
4	GOL	A	705	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21756 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 MYO-INOSITOL PHOSPHOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total 4806	C 3065	N 833	O 887	S 21	0	1	0
1	B	590	Total 4806	C 3065	N 833	O 887	S 21	0	1	0
1	C	590	Total 4806	C 3065	N 833	O 887	S 21	0	1	0
1	D	590	Total 4806	C 3065	N 833	O 887	S 21	0	1	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP A3QMF6
A	10	GLY	-	expression tag	UNP A3QMF6
A	11	SER	-	expression tag	UNP A3QMF6
A	12	SER	-	expression tag	UNP A3QMF6
A	13	HIS	-	expression tag	UNP A3QMF6
A	14	HIS	-	expression tag	UNP A3QMF6
A	15	HIS	-	expression tag	UNP A3QMF6
A	16	HIS	-	expression tag	UNP A3QMF6
A	17	HIS	-	expression tag	UNP A3QMF6
A	18	HIS	-	expression tag	UNP A3QMF6
A	19	SER	-	expression tag	UNP A3QMF6
A	20	SER	-	expression tag	UNP A3QMF6
A	21	GLY	-	expression tag	UNP A3QMF6
A	22	LEU	-	expression tag	UNP A3QMF6
A	23	VAL	-	expression tag	UNP A3QMF6
A	24	PRO	-	expression tag	UNP A3QMF6
A	25	ARG	-	expression tag	UNP A3QMF6
A	26	GLY	-	expression tag	UNP A3QMF6
A	27	SER	-	expression tag	UNP A3QMF6
A	28	HIS	-	expression tag	UNP A3QMF6
A	29	MET	-	expression tag	UNP A3QMF6

Continued on next page...

Continued from previous page...
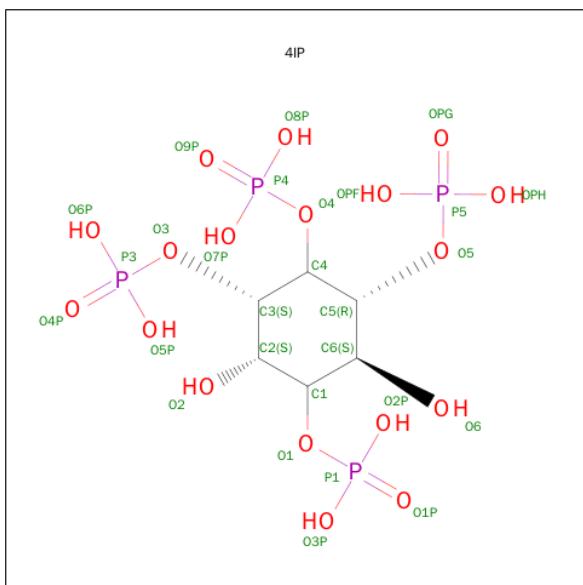
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ALA	-	expression tag	UNP A3QMF6
A	31	SER	-	expression tag	UNP A3QMF6
A	250	SER	CYS	engineered mutation	UNP A3QMF6
A	548	SER	CYS	engineered mutation	UNP A3QMF6
B	9	MET	-	initiating methionine	UNP A3QMF6
B	10	GLY	-	expression tag	UNP A3QMF6
B	11	SER	-	expression tag	UNP A3QMF6
B	12	SER	-	expression tag	UNP A3QMF6
B	13	HIS	-	expression tag	UNP A3QMF6
B	14	HIS	-	expression tag	UNP A3QMF6
B	15	HIS	-	expression tag	UNP A3QMF6
B	16	HIS	-	expression tag	UNP A3QMF6
B	17	HIS	-	expression tag	UNP A3QMF6
B	18	HIS	-	expression tag	UNP A3QMF6
B	19	SER	-	expression tag	UNP A3QMF6
B	20	SER	-	expression tag	UNP A3QMF6
B	21	GLY	-	expression tag	UNP A3QMF6
B	22	LEU	-	expression tag	UNP A3QMF6
B	23	VAL	-	expression tag	UNP A3QMF6
B	24	PRO	-	expression tag	UNP A3QMF6
B	25	ARG	-	expression tag	UNP A3QMF6
B	26	GLY	-	expression tag	UNP A3QMF6
B	27	SER	-	expression tag	UNP A3QMF6
B	28	HIS	-	expression tag	UNP A3QMF6
B	29	MET	-	expression tag	UNP A3QMF6
B	30	ALA	-	expression tag	UNP A3QMF6
B	31	SER	-	expression tag	UNP A3QMF6
B	250	SER	CYS	engineered mutation	UNP A3QMF6
B	548	SER	CYS	engineered mutation	UNP A3QMF6
C	9	MET	-	initiating methionine	UNP A3QMF6
C	10	GLY	-	expression tag	UNP A3QMF6
C	11	SER	-	expression tag	UNP A3QMF6
C	12	SER	-	expression tag	UNP A3QMF6
C	13	HIS	-	expression tag	UNP A3QMF6
C	14	HIS	-	expression tag	UNP A3QMF6
C	15	HIS	-	expression tag	UNP A3QMF6
C	16	HIS	-	expression tag	UNP A3QMF6
C	17	HIS	-	expression tag	UNP A3QMF6
C	18	HIS	-	expression tag	UNP A3QMF6
C	19	SER	-	expression tag	UNP A3QMF6
C	20	SER	-	expression tag	UNP A3QMF6
C	21	GLY	-	expression tag	UNP A3QMF6

Continued on next page...

Continued from previous page...
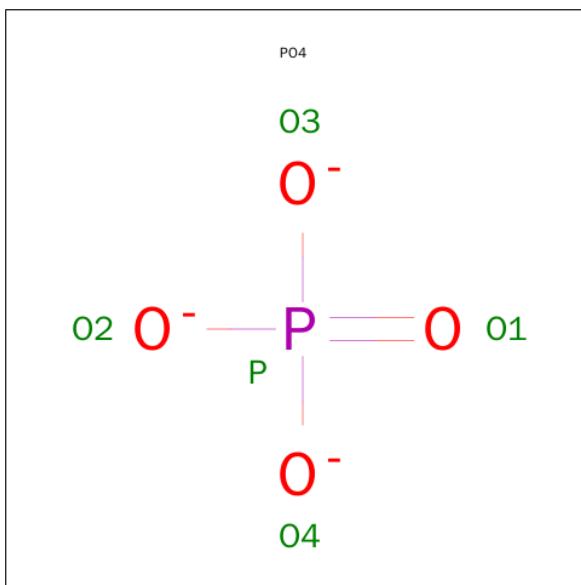
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	LEU	-	expression tag	UNP A3QMF6
C	23	VAL	-	expression tag	UNP A3QMF6
C	24	PRO	-	expression tag	UNP A3QMF6
C	25	ARG	-	expression tag	UNP A3QMF6
C	26	GLY	-	expression tag	UNP A3QMF6
C	27	SER	-	expression tag	UNP A3QMF6
C	28	HIS	-	expression tag	UNP A3QMF6
C	29	MET	-	expression tag	UNP A3QMF6
C	30	ALA	-	expression tag	UNP A3QMF6
C	31	SER	-	expression tag	UNP A3QMF6
C	250	SER	CYS	engineered mutation	UNP A3QMF6
C	548	SER	CYS	engineered mutation	UNP A3QMF6
D	9	MET	-	initiating methionine	UNP A3QMF6
D	10	GLY	-	expression tag	UNP A3QMF6
D	11	SER	-	expression tag	UNP A3QMF6
D	12	SER	-	expression tag	UNP A3QMF6
D	13	HIS	-	expression tag	UNP A3QMF6
D	14	HIS	-	expression tag	UNP A3QMF6
D	15	HIS	-	expression tag	UNP A3QMF6
D	16	HIS	-	expression tag	UNP A3QMF6
D	17	HIS	-	expression tag	UNP A3QMF6
D	18	HIS	-	expression tag	UNP A3QMF6
D	19	SER	-	expression tag	UNP A3QMF6
D	20	SER	-	expression tag	UNP A3QMF6
D	21	GLY	-	expression tag	UNP A3QMF6
D	22	LEU	-	expression tag	UNP A3QMF6
D	23	VAL	-	expression tag	UNP A3QMF6
D	24	PRO	-	expression tag	UNP A3QMF6
D	25	ARG	-	expression tag	UNP A3QMF6
D	26	GLY	-	expression tag	UNP A3QMF6
D	27	SER	-	expression tag	UNP A3QMF6
D	28	HIS	-	expression tag	UNP A3QMF6
D	29	MET	-	expression tag	UNP A3QMF6
D	30	ALA	-	expression tag	UNP A3QMF6
D	31	SER	-	expression tag	UNP A3QMF6
D	250	SER	CYS	engineered mutation	UNP A3QMF6
D	548	SER	CYS	engineered mutation	UNP A3QMF6

- Molecule 2 is INOSITOL-(1,3,4,5)-TETRAKISPHOSPHATE (three-letter code: 4IP) (formula: $C_6H_{16}O_{18}P_4$).
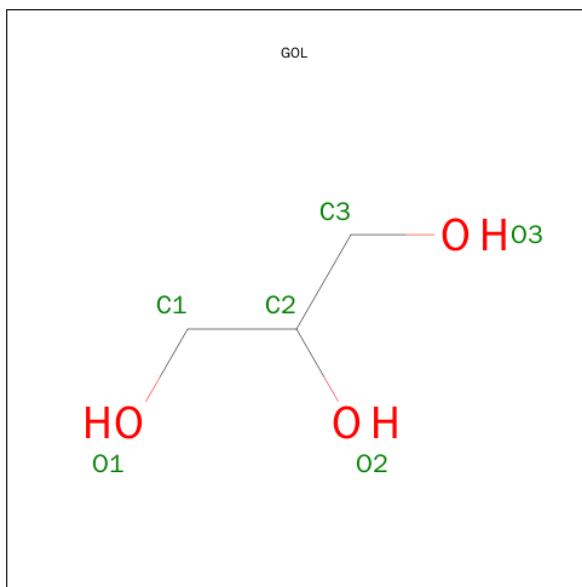
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 28	C 6	O 18	P 4	0	0
2	A	1	Total 28	C 6	O 18	P 4	0	0
2	B	1	Total 28	C 6	O 18	P 4	0	0
2	C	1	Total 28	C 6	O 18	P 4	0	0
2	C	1	Total 28	C 6	O 18	P 4	0	0
2	D	1	Total 28	C 6	O 18	P 4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
3	C	1	Total 5	O 4	P 1	0	0
3	D	1	Total 5	O 4	P 1	0	0
3	D	1	Total 5	O 4	P 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	A	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	B	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	C	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
4	D	1	Total 6	C 3	O 3	0	0
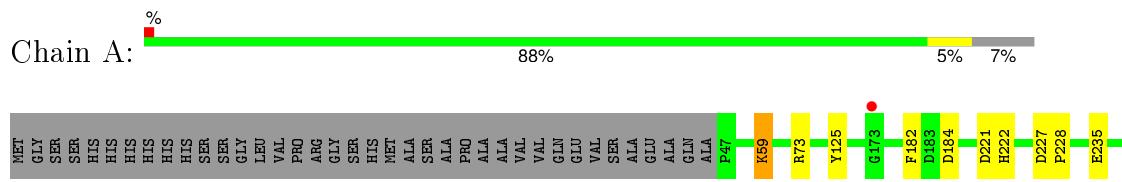
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	578	Total 578	O 578	0	0
5	B	547	Total 547	O 547	0	0
5	C	580	Total 580	O 580	0	0
5	D	557	Total 557	O 557	0	0
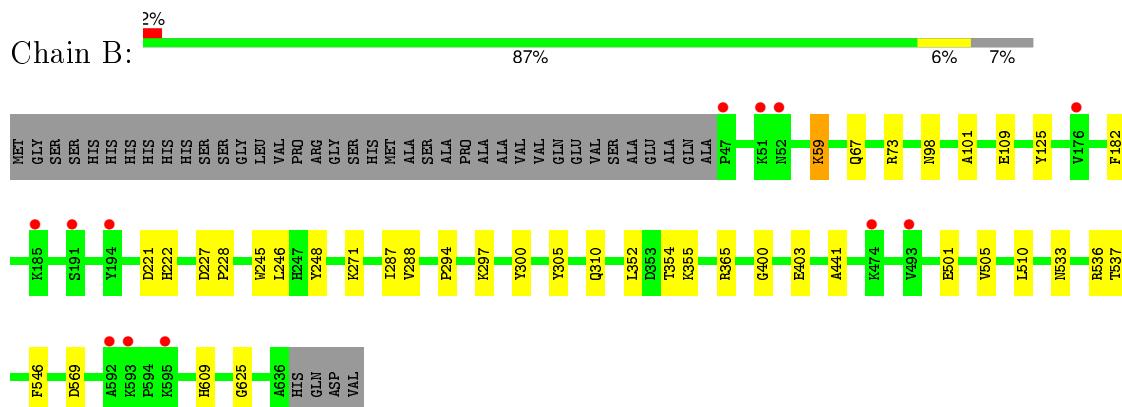
# 3 Residue-property plots ⓘ

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.
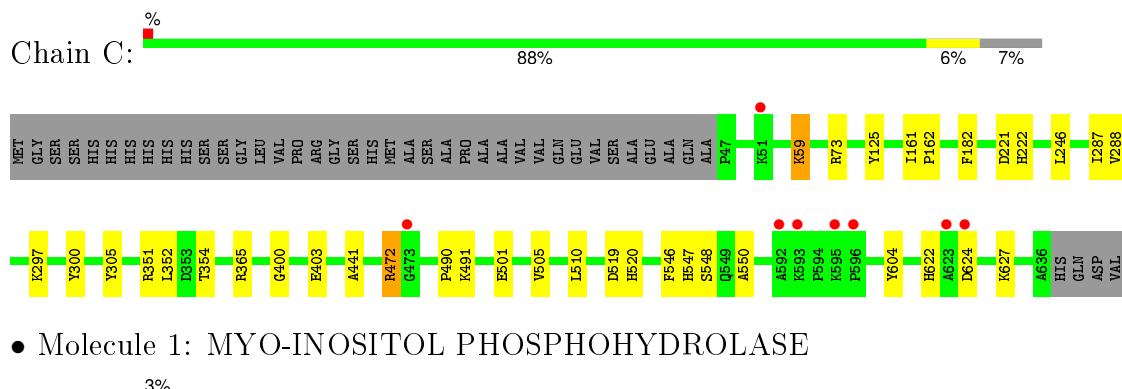
- Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE
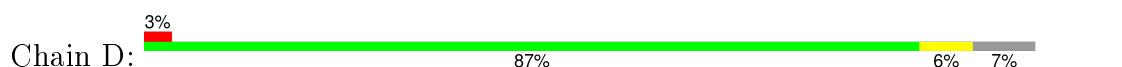
- Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE
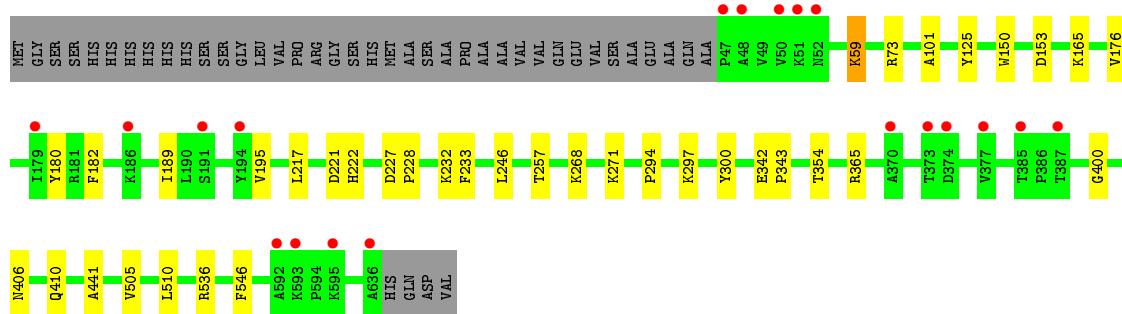
- Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE

- Molecule 1: MYO-INOSITOL PHOSPHOHYDROLASE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.90Å 86.68Å 124.15Å 107.27° 91.69° 90.01°	Depositor
Resolution (Å)	44.54 – 2.20 44.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (44.54-2.20) 88.3 (44.54-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.18 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.190 , 0.213 0.195 , 0.221	Depositor DCC
R_{free} test set	2118 reflections (1.47%)	DCC
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.836	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.3	EDS
Estimated twinning fraction	0.087 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 146418 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21756	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, PO4, 4IP

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	0.37	0/4931	0.54	0/6668
1	B	0.37	0/4931	0.54	0/6668
1	C	0.37	0/4931	0.54	1/6668 (0.0%)
1	D	0.39	0/4931	0.55	0/6668
All	All	0.38	0/19724	0.54	1/26672 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	472	ARG	NE-CZ-NH1	-5.96	117.32	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4806	0	4723	23	0
1	B	4806	0	4723	26	0
1	C	4806	0	4723	27	0
1	D	4806	0	4723	23	0
2	A	56	0	16	4	0
2	B	28	0	8	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	56	0	16	8	0
2	D	28	0	8	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	A	18	0	24	1	0
4	B	18	0	24	0	0
4	C	18	0	24	0	0
4	D	18	0	24	2	0
5	A	578	0	0	3	0
5	B	547	0	0	3	0
5	C	580	0	0	3	0
5	D	557	0	0	3	0
All	All	21756	0	19036	96	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 2.

All (96) 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:B:59:LYS:HE2	1:B:182:PHE:CD1	2.22	0.74
1:B:354:THR:HG22	1:B:441:ALA:HB3	1.72	0.70
1:B:352:LEU:HD21	1:B:355:LYS:HG3	1.74	0.68
1:C:550:ALA:CB	2:C:702:4IP:O2	2.43	0.67
1:D:271:LYS:HE3	5:D:1287:HOH:O	1.98	0.64
1:C:125:TYR:HB2	1:C:246:LEU:HD23	1.82	0.61
1:A:501:GLU:OE2	1:A:547:HIS:NE2	2.33	0.61
1:C:352:LEU:HD22	5:C:1215:HOH:O	2.00	0.60
1:C:550:ALA:HB2	2:C:702:4IP:O2	2.03	0.59
2:C:701:4IP:H2	2:C:701:4IP:O3P	2.03	0.58
1:D:268:LYS:NZ	4:D:705:GOL:H12	2.20	0.57
1:D:268:LYS:HZ3	4:D:705:GOL:H12	1.68	0.57
1:C:604:TYR:OH	2:C:702:4IP:OPF	2.23	0.57
1:B:271:LYS:HE3	5:B:1292:HOH:O	2.05	0.56
1:A:550:ALA:CB	2:A:702:4IP:O2	2.54	0.55
1:A:354:THR:HG22	1:A:441:ALA:HB3	1.87	0.55
1:C:490:PRO:O	1:C:491:LYS:HG2	2.07	0.54
1:C:550:ALA:HB3	2:C:702:4IP:O2	2.06	0.54
1:C:505:VAL:HG13	1:C:510:LEU:HB2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:HIS:CD2	5:B:1187:HOH:O	2.61	0.54
1:C:354:THR:HG22	1:C:441:ALA:HB3	1.89	0.54
1:D:125:TYR:HB2	1:D:246:LEU:HD23	1.91	0.53
1:D:232:LYS:HD2	5:D:932:HOH:O	2.07	0.53
1:B:569:ASP:OD1	1:B:569:ASP:N	2.34	0.53
1:A:235:GLU:HG2	5:A:827:HOH:O	2.09	0.53
1:C:59:LYS:HE2	1:C:182:PHE:CD1	2.44	0.52
1:C:300:TYR:CG	1:D:300:TYR:HB3	2.45	0.52
1:B:294:PRO:HG2	1:B:297:LYS:HG2	1.92	0.52
1:D:59:LYS:HE2	1:D:182:PHE:CD1	2.45	0.51
1:A:125:TYR:HB2	1:A:246:LEU:HD23	1.91	0.51
1:A:300:TYR:HB3	1:B:300:TYR:CG	2.46	0.50
1:B:221:ASP:O	1:B:222:HIS:HB2	2.11	0.50
1:A:244:ALA:HB3	4:A:705:GOL:H32	1.94	0.50
1:A:400:GLY:HA2	1:A:546:PHE:O	2.12	0.50
1:D:354:THR:HG22	1:D:441:ALA:HB3	1.93	0.49
1:A:550:ALA:HB2	2:A:702:4IP:O2	2.13	0.49
1:A:604:TYR:OH	2:A:702:4IP:OPG	2.31	0.49
1:A:221:ASP:O	1:A:222:HIS:HB2	2.12	0.49
1:A:297:LYS:HE2	1:A:305:TYR:CE1	2.48	0.49
1:B:59:LYS:HE2	1:B:182:PHE:CE1	2.48	0.49
1:D:536:ARG:HH11	1:D:536:ARG:HG2	1.78	0.48
1:A:505:VAL:HG13	1:A:510:LEU:HB2	1.95	0.48
1:C:297:LYS:NZ	2:C:701:4IP:O9P	2.34	0.48
1:B:403:GLU:OE1	1:B:501:GLU:OE1	2.32	0.48
1:D:342[B]:GLU:HB2	1:D:343:PRO:HD2	1.96	0.48
1:A:472:ARG:NH1	5:A:821:HOH:O	2.46	0.48
1:C:624:ASP:O	1:C:627:LYS:HG3	2.14	0.48
1:B:287:ILE:HG23	1:B:288:VAL:HG23	1.96	0.47
1:C:300:TYR:HB3	1:D:300:TYR:CG	2.48	0.47
1:B:536:ARG:NH1	1:B:625:GLY:O	2.47	0.47
1:A:287:ILE:HG23	1:A:288:VAL:HG23	1.96	0.47
1:D:180:TYR:HB3	1:D:189:ILE:HG23	1.95	0.47
1:A:550:ALA:HB3	2:A:702:4IP:O2	2.15	0.46
1:B:505:VAL:HG13	1:B:510:LEU:HB2	1.98	0.46
1:C:400:GLY:HA2	1:C:546:PHE:O	2.15	0.46
1:D:294:PRO:HG2	1:D:297:LYS:HG2	1.99	0.45
1:C:472:ARG:NH1	5:C:811:HOH:O	2.40	0.45
1:D:165:LYS:HG3	5:D:888:HOH:O	2.15	0.45
1:C:548:SER:OG	2:C:702:4IP:O2P	2.25	0.45
1:A:300:TYR:CG	1:B:300:TYR:HB3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ARG:NH2	5:A:830:HOH:O	2.50	0.44
1:A:184:ASP:OD1	1:A:251:TYR:OH	2.33	0.44
1:B:400:GLY:HA2	1:B:546:PHE:O	2.17	0.44
1:A:391:LYS:C	1:A:391:LYS:HD3	2.37	0.44
1:B:310:GLN:OE1	5:B:801:HOH:O	2.21	0.44
1:A:403:GLU:OE2	1:A:501:GLU:OE1	2.36	0.44
1:C:351:ARG:NH2	2:C:702:4IP:O6P	2.43	0.43
1:D:400:GLY:HA2	1:D:546:PHE:O	2.18	0.43
1:C:297:LYS:HE2	1:C:305:TYR:CE1	2.53	0.43
1:C:287:ILE:HG23	1:C:288:VAL:HG23	2.00	0.43
1:C:221:ASP:O	1:C:222:HIS:HB2	2.17	0.43
1:C:501:GLU:OE2	1:C:547:HIS:NE2	2.48	0.43
1:B:98:ASN:HA	1:B:245:TRP:CZ3	2.54	0.43
1:A:59:LYS:HE2	1:A:182:PHE:CD1	2.54	0.43
1:B:297:LYS:HE2	1:B:305:TYR:CE1	2.54	0.43
1:B:67:GLN:O	1:B:109:GLU:HA	2.19	0.43
1:D:505:VAL:HG13	1:D:510:LEU:HB2	2.01	0.43
1:C:622:HIS:HE1	5:C:1194:HOH:O	2.01	0.42
1:C:403:GLU:OE1	1:C:501:GLU:OE1	2.38	0.42
1:B:227:ASP:HB2	1:B:228:PRO:HD3	2.02	0.42
1:D:176:VAL:HA	1:D:195:VAL:O	2.19	0.42
1:B:354:THR:CG2	1:B:441:ALA:HB3	2.45	0.42
1:D:101:ALA:HB1	1:D:257:THR:CG2	2.50	0.42
1:D:150:TRP:HB3	1:D:153:ASP:HB2	2.02	0.42
1:B:101:ALA:HA	1:B:248:TYR:O	2.19	0.41
1:B:533:ASN:O	1:B:537:THR:HG22	2.20	0.41
1:C:519:ASP:O	1:C:520:HIS:HB2	2.20	0.41
1:A:227:ASP:HB2	1:A:228:PRO:HD3	2.02	0.41
1:D:227:ASP:HB2	1:D:228:PRO:HD3	2.03	0.41
1:B:125:TYR:HB2	1:B:246:LEU:HD23	2.02	0.41
1:B:221:ASP:O	1:B:222:HIS:CB	2.69	0.41
1:D:221:ASP:O	1:D:222:HIS:HB2	2.21	0.41
1:C:125:TYR:HB2	1:C:246:LEU:CD2	2.48	0.40
1:D:406:ASN:O	1:D:410:GLN:HG2	2.21	0.40
1:D:217:LEU:HD11	1:D:233:PHE:HB2	2.02	0.40
1:C:161:ILE:HB	1:C:162:PRO:CD	2.51	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	589/632 (93%)	572 (97%)	17 (3%)	0	100	100
1	B	589/632 (93%)	573 (97%)	16 (3%)	0	100	100
1	C	589/632 (93%)	571 (97%)	18 (3%)	0	100	100
1	D	589/632 (93%)	572 (97%)	17 (3%)	0	100	100
All	All	2356/2528 (93%)	2288 (97%)	68 (3%)	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	516/547 (94%)	513 (99%)	3 (1%)	90	95
1	B	516/547 (94%)	513 (99%)	3 (1%)	90	95
1	C	516/547 (94%)	513 (99%)	3 (1%)	90	95
1	D	516/547 (94%)	513 (99%)	3 (1%)	90	95
All	All	2064/2188 (94%)	2052 (99%)	12 (1%)	90	95

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

Mol	Chain	Res	Type
1	A	59	LYS
1	A	73	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	365	ARG
1	B	59	LYS
1	B	73	ARG
1	B	365	ARG
1	C	59	LYS
1	C	73	ARG
1	C	365	ARG
1	D	59	LYS
1	D	73	ARG
1	D	365	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	520	HIS
1	B	310	GLN
1	B	622	HIS
1	C	187	ASN
1	C	622	HIS
1	D	187	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

24 ligands are 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	4IP	A	701	-	24,28,28	0.59	0	46,46,46	0.98	0
2	4IP	A	702	-	24,28,28	0.59	0	46,46,46	1.05	0
3	PO4	A	703	-	4,4,4	0.64	0	6,6,6	0.24	0
4	GOL	A	704	-	5,5,5	0.27	0	5,5,5	0.16	0
4	GOL	A	705	-	5,5,5	0.36	0	5,5,5	0.17	0
4	GOL	A	706	-	5,5,5	0.27	0	5,5,5	0.47	0
2	4IP	B	701	-	24,28,28	0.58	0	46,46,46	0.99	1 (2%)
3	PO4	B	702	-	4,4,4	0.56	0	6,6,6	0.24	0
3	PO4	B	703	-	4,4,4	0.82	0	6,6,6	0.25	0
4	GOL	B	704	-	5,5,5	0.16	0	5,5,5	0.31	0
4	GOL	B	705	-	5,5,5	0.38	0	5,5,5	0.31	0
4	GOL	B	706	-	5,5,5	0.27	0	5,5,5	0.24	0
2	4IP	C	701	-	24,28,28	0.61	0	46,46,46	1.01	1 (2%)
2	4IP	C	702	-	24,28,28	0.60	0	46,46,46	1.03	1 (2%)
3	PO4	C	703	-	4,4,4	0.61	0	6,6,6	0.24	0
4	GOL	C	704	-	5,5,5	0.28	0	5,5,5	0.07	0
4	GOL	C	705	-	5,5,5	0.37	0	5,5,5	0.46	0
4	GOL	C	706	-	5,5,5	0.25	0	5,5,5	0.24	0
2	4IP	D	701	-	24,28,28	0.57	0	46,46,46	1.00	0
3	PO4	D	702	-	4,4,4	0.77	0	6,6,6	0.25	0
3	PO4	D	703	-	4,4,4	0.73	0	6,6,6	0.25	0
4	GOL	D	704	-	5,5,5	0.16	0	5,5,5	0.11	0
4	GOL	D	705	-	5,5,5	0.48	0	5,5,5	0.51	0
4	GOL	D	706	-	5,5,5	0.33	0	5,5,5	0.20	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	4IP	A	701	-	-	0/20/44/44	0/1/1/1
2	4IP	A	702	-	-	0/20/44/44	0/1/1/1
3	PO4	A	703	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	704	-	-	0/4/4/4	0/0/0/0
4	GOL	A	705	-	-	0/4/4/4	0/0/0/0
4	GOL	A	706	-	-	0/4/4/4	0/0/0/0
2	4IP	B	701	-	-	0/20/44/44	0/1/1/1
3	PO4	B	702	-	-	0/0/0/0	0/0/0/0
3	PO4	B	703	-	-	0/0/0/0	0/0/0/0
4	GOL	B	704	-	-	0/4/4/4	0/0/0/0
4	GOL	B	705	-	-	0/4/4/4	0/0/0/0
4	GOL	B	706	-	-	0/4/4/4	0/0/0/0
2	4IP	C	701	-	-	0/20/44/44	0/1/1/1
2	4IP	C	702	-	-	0/20/44/44	0/1/1/1
3	PO4	C	703	-	-	0/0/0/0	0/0/0/0
4	GOL	C	704	-	-	0/4/4/4	0/0/0/0
4	GOL	C	705	-	-	0/4/4/4	0/0/0/0
4	GOL	C	706	-	-	0/4/4/4	0/0/0/0
2	4IP	D	701	-	-	0/20/44/44	0/1/1/1
3	PO4	D	702	-	-	0/0/0/0	0/0/0/0
3	PO4	D	703	-	-	0/0/0/0	0/0/0/0
4	GOL	D	704	-	-	0/4/4/4	0/0/0/0
4	GOL	D	705	-	-	0/4/4/4	0/0/0/0
4	GOL	D	706	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	4IP	O3P-P1-O2P	2.06	114.99	107.44
2	C	702	4IP	O8P-P4-O7P	2.12	115.24	107.44
2	C	701	4IP	O8P-P4-O7P	2.22	115.60	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	4IP	4	0
4	A	705	GOL	1	0
2	C	701	4IP	2	0
2	C	702	4IP	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	705	GOL	2	0

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(Å²)	Q<0.9
1	A	590/632 (93%)	-0.23	8 (1%)	78	77	5, 14, 35, 62	0
1	B	590/632 (93%)	-0.04	12 (2%)	68	67	5, 17, 39, 72	0
1	C	590/632 (93%)	-0.15	8 (1%)	78	77	6, 14, 35, 62	0
1	D	590/632 (93%)	0.04	19 (3%)	51	50	7, 17, 41, 70	0
All	All	2360/2528 (93%)	-0.09	47 (1%)	68	67	5, 16, 38, 72	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	592	ALA	6.5
1	C	592	ALA	4.7
1	D	373	THR	4.2
1	A	592	ALA	4.2
1	B	51	LYS	4.1
1	B	593	LYS	4.0
1	D	636	ALA	4.0
1	D	47	PRO	3.8
1	D	592	ALA	3.7
1	C	593	LYS	3.6
1	D	51	LYS	3.6
1	A	173	GLY	3.2
1	D	593	LYS	3.2
1	D	191	SER	3.2
1	B	191	SER	2.8
1	C	623	ALA	2.7
1	B	47	PRO	2.7
1	C	595	LYS	2.7
1	D	377	VAL	2.7
1	A	593	LYS	2.6
1	D	370	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	52	ASN	2.6
1	D	179	ILE	2.6
1	A	627	LYS	2.5
1	C	51	LYS	2.5
1	C	473	GLY	2.5
1	D	50	VAL	2.5
1	A	373	THR	2.4
1	B	194	TYR	2.4
1	D	387	THR	2.4
1	C	596	PRO	2.4
1	D	48	ALA	2.3
1	B	595	LYS	2.2
1	A	635	ALA	2.2
1	B	185	LYS	2.2
1	B	52	ASN	2.1
1	B	176	VAL	2.1
1	D	186	LYS	2.1
1	A	596	PRO	2.1
1	A	377	VAL	2.1
1	D	374	ASP	2.1
1	C	624	ASP	2.1
1	D	385	THR	2.1
1	B	493	VAL	2.0
1	D	194	TYR	2.0
1	B	474	LYS	2.0
1	D	595	LYS	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)

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	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	4IP	B	701	28/28	0.80	0.24	4.93	31,48,60,64	28
2	4IP	A	701	28/28	0.81	0.27	3.67	36,54,61,62	28
2	4IP	C	701	28/28	0.83	0.24	2.98	42,52,61,63	28
4	GOL	A	705	6/6	0.84	0.21	2.93	21,26,29,31	0
2	4IP	A	702	28/28	0.91	0.24	2.80	17,50,71,79	0
2	4IP	C	702	28/28	0.92	0.25	2.65	17,58,78,86	0
4	GOL	C	705	6/6	0.87	0.17	1.92	23,28,29,31	0
4	GOL	D	705	6/6	0.81	0.20	1.57	27,31,34,34	0
2	4IP	D	701	28/28	0.84	0.23	1.50	34,45,51,54	28
4	GOL	B	704	6/6	0.92	0.15	1.46	20,22,24,28	0
4	GOL	B	705	6/6	0.83	0.18	1.44	28,36,39,41	0
4	GOL	A	704	6/6	0.92	0.14	0.65	18,19,20,21	0
3	PO4	D	702	5/5	0.98	0.12	0.43	12,14,17,18	0
4	GOL	D	704	6/6	0.92	0.14	0.16	14,16,17,18	0
3	PO4	B	703	5/5	0.98	0.12	-0.81	11,11,12,12	0
3	PO4	A	703	5/5	0.98	0.10	-0.87	10,11,12,13	0
4	GOL	C	704	6/6	0.96	0.12	-0.89	14,17,18,19	0
3	PO4	D	703	5/5	0.98	0.10	-0.98	8,8,9,10	0
3	PO4	C	703	5/5	0.99	0.10	-1.92	10,11,11,11	0
3	PO4	B	702	5/5	0.98	0.07	-3.25	11,14,15,17	0
4	GOL	C	706	6/6	0.88	0.17	-	16,20,22,26	0
4	GOL	B	706	6/6	0.89	0.16	-	19,21,24,24	0
4	GOL	D	706	6/6	0.90	0.19	-	20,23,24,26	0
4	GOL	A	706	6/6	0.90	0.17	-	18,22,23,26	0

6.5 Other polymers (i)

There are no such residues in this entry.