Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:10 PM GMT

PDB ID	:	4KQM
Title	:	Crystal structure of yeast glycogen synthase E169Q mutant in complex with glucose and UDP
Authors	:	Chikwana, V.M.; Hurley, T.D.
Deposited on	:	2013-05-15
Resolution	:	2.77 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:

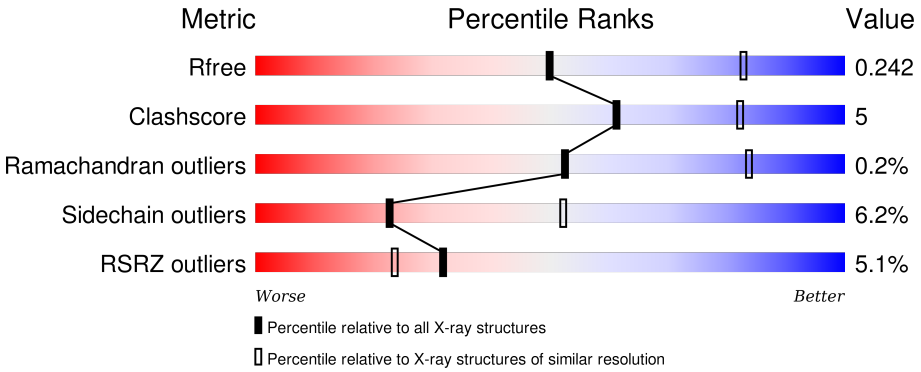
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.77 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	3004 (2.80-2.76)
Clashscore	102246	3480 (2.80-2.76)
Ramachandran outliers	100387	3423 (2.80-2.76)
Sidechain outliers	100360	3425 (2.80-2.76)
RSRZ outliers	91569	3016 (2.80-2.76)

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	724	4% 73% 14% • 12%
1	B	724	2% 72% 15% • 12%
1	C	724	5% 72% 15% • 12%
1	D	724	7% 72% 15% • 12%

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
4	PEG	B	803	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20825 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 Gsy2p.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	B	638	Total	C	N	O	S	0	1	0
			5163	3296	904	944	19			
1	C	638	Total	C	N	O	S	0	0	0
			5157	3292	903	943	19			
1	D	635	Total	C	N	O	S	0	0	0
			5132	3276	900	937	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
A	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
A	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
A	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
A	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
A	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
A	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
A	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
A	0	SER	-	EXPRESSION TAG	UNP E7NKU1
A	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
B	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
B	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
B	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
B	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
B	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
B	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
B	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
B	0	SER	-	EXPRESSION TAG	UNP E7NKU1
B	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
C	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
C	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-16	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
C	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
C	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
C	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
C	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
C	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
C	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
C	0	SER	-	EXPRESSION TAG	UNP E7NKU1
C	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1
D	-18	MET	-	INITIATING METHIONINE	UNP E7NKU1
D	-17	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-16	SER	-	EXPRESSION TAG	UNP E7NKU1

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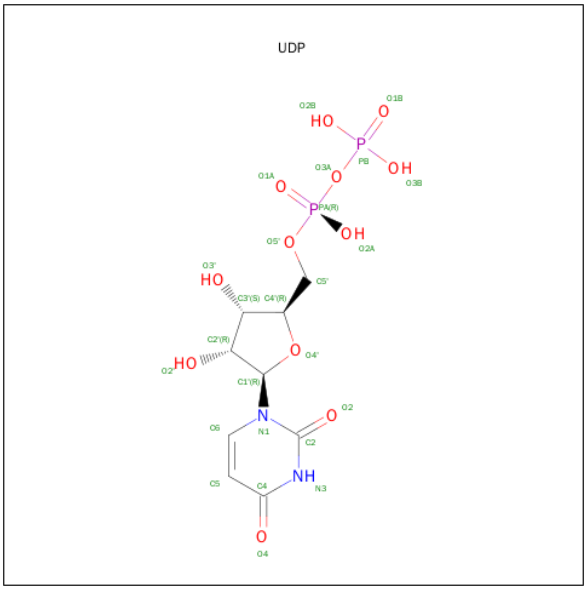
Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-14	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-13	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-12	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-11	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-10	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-9	HIS	-	EXPRESSION TAG	UNP E7NKU1
D	-8	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-7	SER	-	EXPRESSION TAG	UNP E7NKU1
D	-6	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	-5	LEU	-	EXPRESSION TAG	UNP E7NKU1
D	-4	VAL	-	EXPRESSION TAG	UNP E7NKU1
D	-3	PRO	-	EXPRESSION TAG	UNP E7NKU1
D	-2	ARG	-	EXPRESSION TAG	UNP E7NKU1
D	-1	GLY	-	EXPRESSION TAG	UNP E7NKU1
D	0	SER	-	EXPRESSION TAG	UNP E7NKU1
D	169	GLN	GLU	ENGINEERED MUTATION	UNP E7NKU1

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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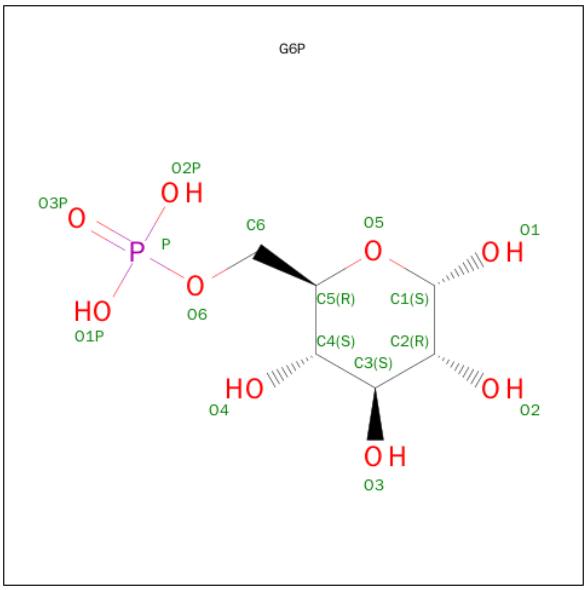
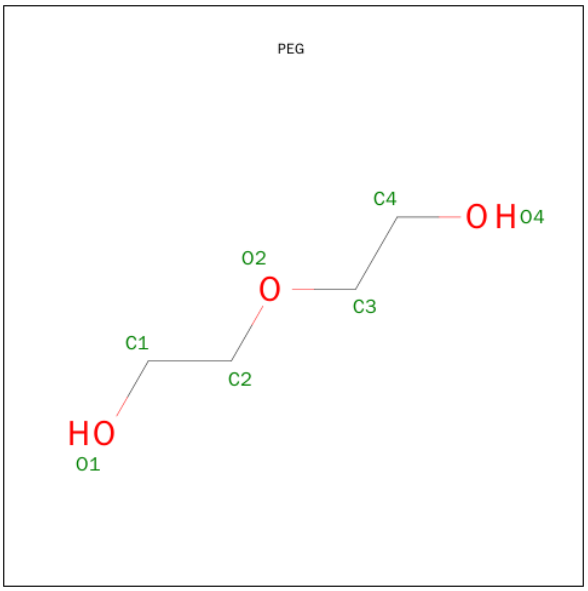
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	O	P		0	0
			16	6	9	1			
3	B	1	Total	C	O	P		0	0
			16	6	9	1			
3	C	1	Total	C	O	P		0	0
			16	6	9	1			
3	D	1	Total	C	O	P		0	0
			16	6	9	1			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	B	1	Total C O 7 4 3	0	0
4	C	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

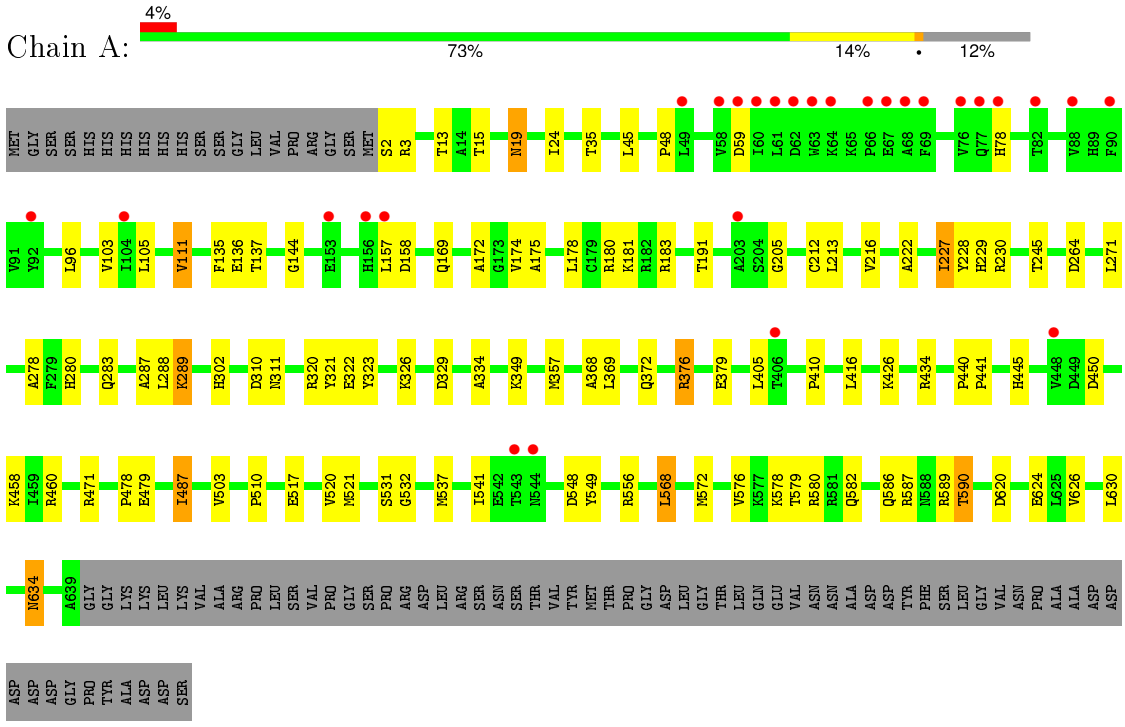
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	2	Total C O 24 12 12	0	0

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.

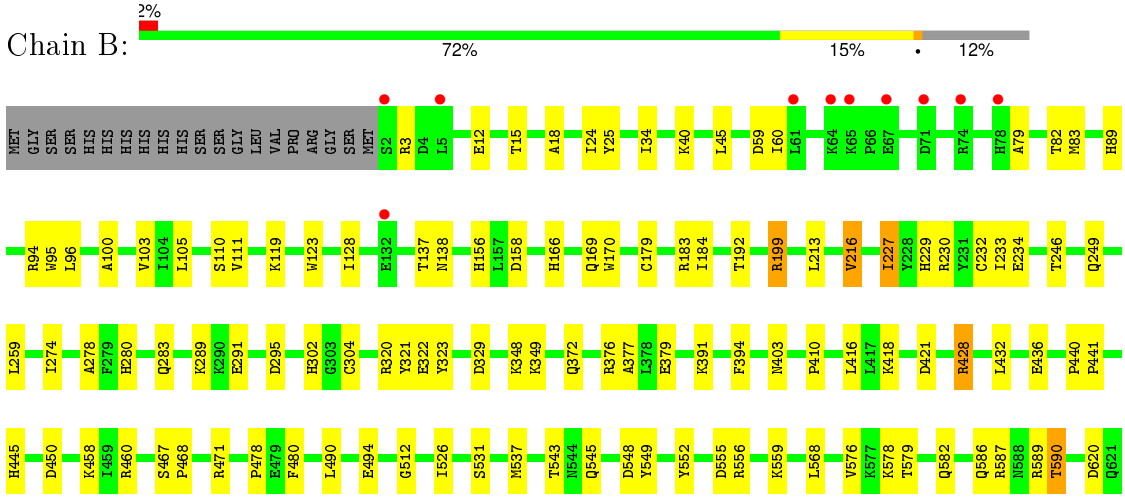
- Molecule 1: Gsy2p

Chain A:



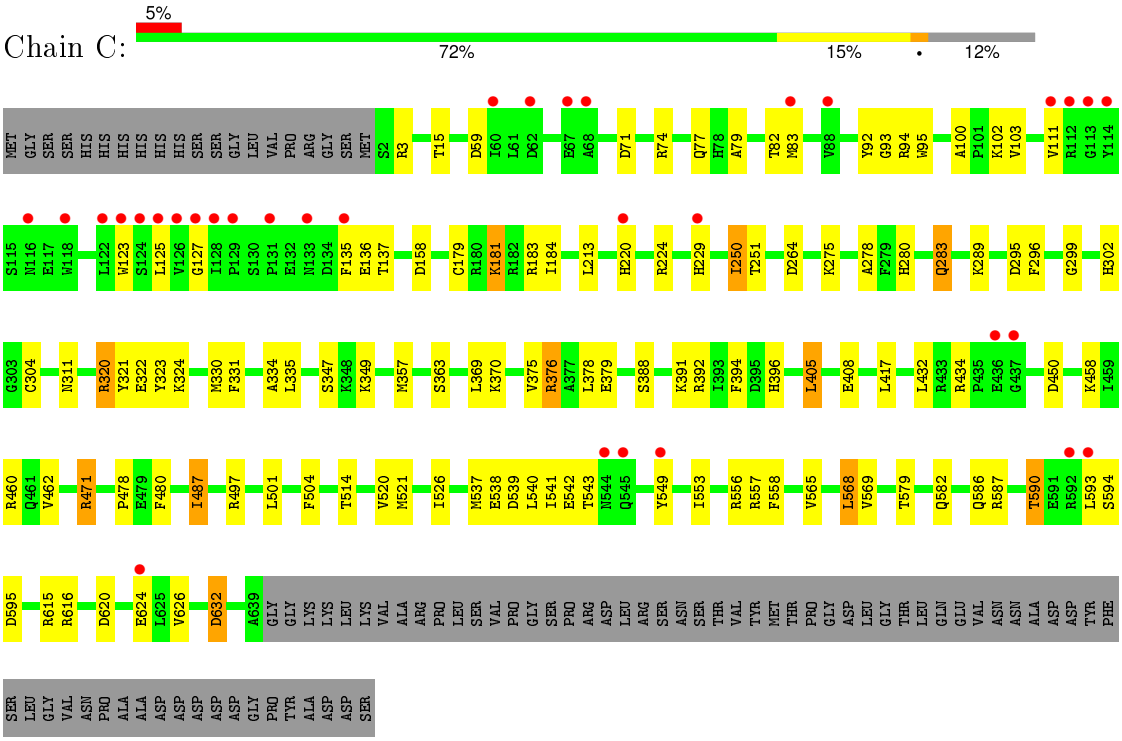
- Molecule 1: Gsy2p

Chain B:



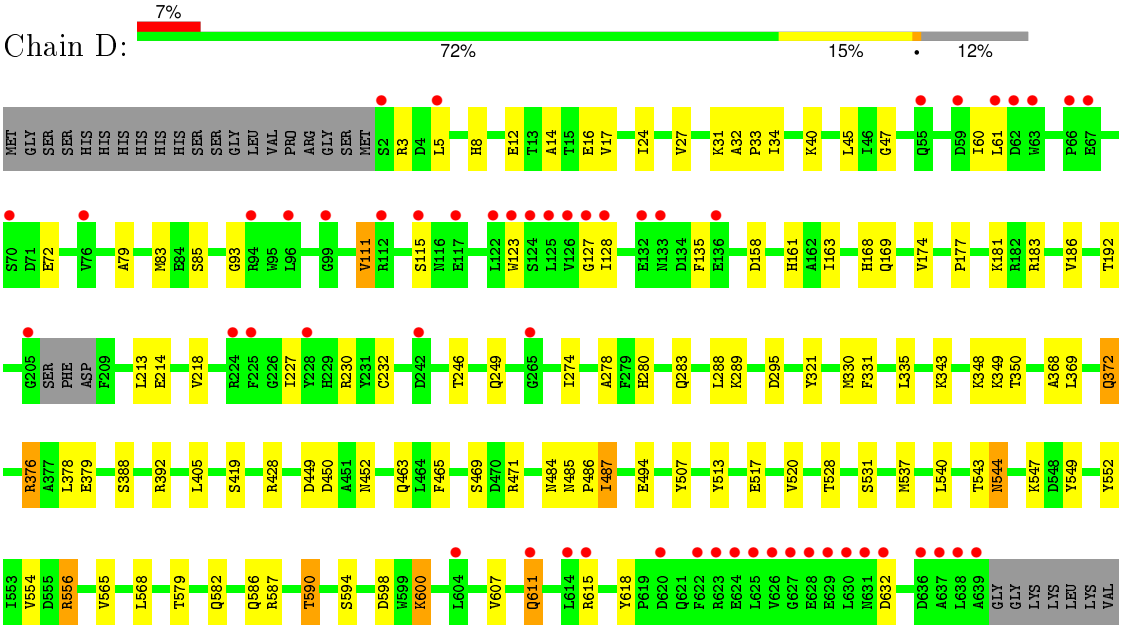
• Molecule 1: Gsy2p

Chain C:



• Molecule 1: Gsy2p

Chain D:



ALA ARG PRO LEU SER VAL PRO GLY SER PRO ARG ASP LEU ARG SER ASN SER THR VAL TYR MET THR PRO GLY ASP LEU GLY THR LEU GLN GLU VAL ASN ASN ALA ASP ASP TYR PHE SER LEU GLY VAL ASN PRO ALA ALA ASP ASP ASP ASP ASP GLY PRO TYR ALA ASP ASP SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	192.71Å 204.44Å 206.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.77 48.41 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.41-2.77) 98.7 (48.41-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.201 , 0.241 0.201 , 0.242	Depositor DCC
R_{free} test set	5073 reflections (5.23%)	DCC
Wilson B-factor (Å^2)	53.7	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.8	EDS
Estimated twinning fraction	0.005 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 102101 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	20825	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, UDP, BGC, PEG, G6P

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	0.42	0/5282	0.59	0/7155
1	B	0.51	0/5291	0.67	0/7167
1	C	0.44	0/5282	0.61	0/7155
1	D	0.45	0/5255	0.59	0/7117
All	All	0.46	0/21110	0.62	0/28594

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	5157	0	5072	60	0
1	B	5163	0	5080	57	0
1	C	5157	0	5072	64	0
1	D	5132	0	5053	54	1
2	A	25	0	11	0	0
2	B	25	0	11	1	0
2	C	25	0	11	3	0
2	D	25	0	11	0	0
3	A	16	0	11	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	16	0	11	1	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
4	A	7	0	10	1	0
4	B	7	0	10	1	0
4	C	7	0	10	2	0
4	D	7	0	10	1	0
5	C	24	0	12	0	0
All	All	20825	0	20417	226	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 (226) 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:283:GLN:HG2	1:C:280:HIS:CE1	2.00	0.96
1:A:280:HIS:CE1	1:D:283:GLN:HG2	2.07	0.88
1:B:280:HIS:CE1	1:C:283:GLN:HG2	2.10	0.86
1:A:379:GLU:HG2	4:B:803:PEG:H41	1.65	0.78
1:B:349:LYS:HE2	1:B:576:VAL:O	1.85	0.77
1:A:586:GLN:O	1:A:590:THR:HG22	1.85	0.76
1:A:283:GLN:HG2	1:D:280:HIS:CE1	2.21	0.75
1:B:199:ARG:HG2	1:B:199:ARG:HH11	1.52	0.74
1:B:192:THR:HG22	1:B:246:THR:HG22	1.69	0.74
1:D:586:GLN:O	1:D:590:THR:HG22	1.87	0.74
1:A:19:ASN:HD22	1:A:19:ASN:H	1.40	0.69
1:A:320:ARG:HG3	1:A:326:LYS:HD2	1.73	0.69
1:C:320:ARG:NH2	1:C:322:GLU:OE2	2.25	0.69
1:D:543:THR:O	1:D:544:ASN:HB2	1.92	0.69
1:C:520:VAL:HA	1:C:594:SER:HB3	1.76	0.68
1:B:199:ARG:CG	1:B:199:ARG:HH11	2.07	0.68
1:C:586:GLN:O	1:C:590:THR:HG22	1.93	0.68
1:A:280:HIS:CE1	1:D:283:GLN:CG	2.77	0.67
1:C:391:LYS:HD3	4:C:805:PEG:H41	1.76	0.67
1:B:128:ILE:HG12	1:B:232:CYS:HB3	1.78	0.66
1:B:94:ARG:HD2	1:B:100:ALA:HB1	1.79	0.65
1:A:19:ASN:N	1:A:19:ASN:HD22	1.94	0.64
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.29	0.64
1:B:192:THR:CG2	1:B:246:THR:HG22	2.28	0.63
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD11	1:A:169:GLN:CG	2.29	0.63
1:B:579:THR:H	1:B:582:GLN:NE2	1.97	0.62
1:C:379:GLU:HG2	4:D:803:PEG:H11	1.83	0.61
1:C:378:LEU:HD22	1:C:432:LEU:HD11	1.83	0.61
1:A:283:GLN:HG3	3:A:802:G6P:O1	2.01	0.60
1:B:377:ALA:HB1	1:B:428:ARG:NH1	2.16	0.60
1:A:24:ILE:HD11	1:A:169:GLN:HG3	1.83	0.59
1:C:587:ARG:HA	1:C:590:THR:HG23	1.83	0.59
1:D:579:THR:H	1:D:582:GLN:NE2	2.01	0.59
1:A:369:LEU:HA	1:A:487:ILE:HD11	1.85	0.58
1:B:548:ASP:O	1:B:589:ARG:NH1	2.31	0.58
1:B:586:GLN:O	1:B:590:THR:HG22	2.03	0.58
1:C:304:CYS:SG	1:C:434:ARG:HD3	2.43	0.58
1:D:598:ASP:OD2	1:D:600:LYS:HB2	2.03	0.58
1:D:61:LEU:HD12	1:D:93:GLY:HA2	1.86	0.57
1:B:227:ILE:HD12	1:B:230:ARG:HD2	1.86	0.56
1:B:18:ALA:HB2	1:B:105:LEU:HD22	1.86	0.56
4:A:803:PEG:H12	1:B:379:GLU:HG2	1.88	0.56
1:B:549:TYR:O	1:B:590:THR:HB	2.06	0.56
1:D:513:TYR:O	1:D:517:GLU:HB2	2.06	0.56
1:A:549:TYR:O	1:A:590:THR:HB	2.06	0.55
1:D:579:THR:H	1:D:582:GLN:HE21	1.52	0.55
1:D:549:TYR:O	1:D:590:THR:HB	2.05	0.55
1:B:89:HIS:HD2	1:B:110:SER:HB2	1.72	0.54
1:B:410:PRO:HG2	1:B:416:LEU:HD21	1.89	0.54
1:A:579:THR:H	1:A:582:GLN:NE2	2.06	0.54
1:A:175:ALA:HA	1:A:178:LEU:HD12	1.90	0.54
1:A:264:ASP:O	1:A:634:ASN:HB2	2.08	0.54
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.90	0.53
1:D:227:ILE:HG13	1:D:230:ARG:HD2	1.90	0.53
1:B:320:ARG:HG3	1:B:322:GLU:HG3	1.91	0.53
1:A:103:VAL:HG12	1:A:105:LEU:HG	1.90	0.53
1:D:547:LYS:HG2	1:D:552:TYR:CD1	2.44	0.52
1:D:372:GLN:NE2	1:D:486:PRO:O	2.42	0.52
1:C:320:ARG:NH1	2:C:803:UDP:O3B	2.43	0.52
1:B:213:LEU:HA	1:B:216:VAL:HG13	1.92	0.51
1:D:368:ALA:O	1:D:487:ILE:HD11	2.09	0.51
1:D:27:VAL:O	1:D:31:LYS:HB2	2.10	0.51
1:D:388:SER:HB3	1:D:392:ARG:NH1	2.26	0.51
1:A:372:GLN:NE2	1:A:376:ARG:HH11	2.08	0.51
1:A:357:MET:O	1:A:478:PRO:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ILE:HD11	1:A:169:GLN:HG2	1.92	0.50
1:C:620:ASP:O	1:C:624:GLU:HG2	2.10	0.50
1:D:3:ARG:NH2	1:D:158:ASP:O	2.45	0.50
1:D:5:LEU:O	1:D:8:HIS:HD2	1.94	0.50
1:A:334:ALA:CB	1:A:568:LEU:HD13	2.41	0.50
1:B:179:CYS:HA	1:B:184:ILE:HD12	1.93	0.50
1:D:349:LYS:O	1:D:471:ARG:HD3	2.12	0.50
1:D:123:TRP:O	1:D:127:GLY:HA2	2.11	0.50
1:B:620:ASP:O	1:B:624:GLU:HG2	2.12	0.50
1:D:449:ASP:OD2	1:D:452:ASN:HB2	2.11	0.50
1:C:579:THR:H	1:C:582:GLN:NE2	2.09	0.50
1:C:450:ASP:OD1	1:C:460:ARG:NH2	2.45	0.49
1:C:579:THR:H	1:C:582:GLN:HE21	1.58	0.49
1:A:78:HIS:HB3	1:A:157:LEU:HD13	1.93	0.49
1:A:410:PRO:HG2	1:A:416:LEU:HD21	1.94	0.49
1:B:579:THR:H	1:B:582:GLN:HE21	1.59	0.49
1:A:302:HIS:O	1:A:434:ARG:HD2	2.12	0.49
1:C:95:TRP:HB2	1:C:103:VAL:HG21	1.95	0.49
1:C:92:TYR:OH	1:C:102:LYS:HD2	2.12	0.48
1:C:137:THR:HG21	1:C:229:HIS:CD2	2.48	0.48
1:D:520:VAL:HA	1:D:594:SER:HB2	1.94	0.48
1:D:295:ASP:CG	1:D:376:ARG:HH22	2.17	0.48
1:A:227:ILE:HD12	1:A:230:ARG:HD2	1.96	0.48
1:B:349:LYS:O	1:B:471:ARG:HD3	2.13	0.48
1:D:587:ARG:HA	1:D:590:THR:HG23	1.96	0.48
1:A:289:LYS:N	1:A:289:LYS:HD2	2.29	0.48
1:A:580:ARG:HE	3:A:802:G6P:H62	1.78	0.48
1:C:250:ILE:HG22	1:C:251:THR:N	2.29	0.48
1:C:538:GLU:HG3	1:C:553:ILE:HD13	1.95	0.48
1:D:368:ALA:C	1:D:487:ILE:HD11	2.35	0.47
1:A:191:THR:OG1	1:A:245:THR:OG1	2.31	0.47
1:B:490:LEU:HD22	1:B:494:GLU:HB3	1.95	0.47
1:C:59:ASP:O	1:C:93:GLY:HA3	2.14	0.47
1:B:555:ASP:HB3	1:B:559:LYS:HD2	1.97	0.47
1:A:368:ALA:O	1:A:487:ILE:HD11	2.14	0.47
1:B:59:ASP:HB2	1:B:96:LEU:HD21	1.96	0.47
1:A:626:VAL:HG11	1:A:630:LEU:HD11	1.95	0.47
1:B:283:GLN:CG	1:C:280:HIS:CE1	2.88	0.47
1:B:199:ARG:CG	1:B:199:ARG:NH1	2.70	0.47
1:A:13:THR:HG22	1:A:172:ALA:HB1	1.95	0.47
1:B:103:VAL:HG12	1:B:105:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:PHE:CZ	1:C:335:LEU:HD11	2.49	0.47
1:B:445:HIS:ND1	1:B:478:PRO:HD2	2.29	0.47
1:A:222:ALA:HB1	1:A:228:TYR:HA	1.97	0.47
1:C:3:ARG:NH2	1:C:158:ASP:O	2.47	0.47
1:D:174:VAL:O	1:D:177:PRO:HD2	2.15	0.47
1:A:144:GLY:HA3	1:A:174:VAL:HB	1.97	0.47
1:A:572:MET:O	1:A:576:VAL:HG23	2.14	0.47
1:D:24:ILE:HD11	1:D:169:GLN:HG3	1.97	0.47
1:A:278:ALA:HB1	1:A:280:HIS:CE1	2.50	0.47
1:C:311:ASN:OD1	1:C:349:LYS:NZ	2.46	0.47
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.50	0.46
1:B:578:LYS:HA	1:B:582:GLN:NE2	2.30	0.46
1:A:372:GLN:HE21	1:A:376:ARG:NH1	2.12	0.46
1:A:548:ASP:O	1:A:589:ARG:NH1	2.43	0.46
1:B:3:ARG:NH2	1:B:158:ASP:O	2.48	0.46
1:C:458:LYS:O	1:C:462:VAL:HG22	2.15	0.46
1:B:480:PHE:CD1	2:B:801:UDP:C4	3.03	0.46
1:D:5:LEU:HD21	1:D:618:TYR:HD1	1.81	0.46
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.31	0.46
1:D:607:VAL:O	1:D:611:GLN:HG2	2.15	0.46
1:A:620:ASP:O	1:A:624:GLU:HG2	2.16	0.46
1:B:95:TRP:HB2	1:B:103:VAL:HG21	1.98	0.46
1:B:103:VAL:CG1	1:B:105:LEU:HG	2.46	0.46
1:C:504:PHE:CE1	1:C:514:THR:CG2	2.99	0.46
1:D:543:THR:O	1:D:544:ASN:CB	2.62	0.46
1:A:372:GLN:HE21	1:A:376:ARG:HH11	1.62	0.46
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.98	0.46
1:C:370:LYS:HB3	1:C:370:LYS:HE2	1.78	0.46
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.98	0.46
1:B:467:SER:HB2	1:B:468:PRO:HD2	1.97	0.46
1:A:311:ASN:OD1	1:A:349:LYS:HD3	2.16	0.46
1:A:578:LYS:HA	1:A:582:GLN:NE2	2.31	0.45
1:B:283:GLN:HG3	3:B:802:G6P:O1	2.16	0.45
1:C:394:PHE:CE1	1:D:379:GLU:HG3	2.51	0.45
1:C:125:LEU:HD22	1:C:181:LYS:HD2	1.99	0.45
1:B:526:ILE:HG12	1:B:552:TYR:HB2	1.97	0.45
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.51	0.45
1:B:587:ARG:HA	1:B:590:THR:CG2	2.47	0.45
1:A:19:ASN:ND2	1:A:19:ASN:N	2.63	0.45
1:C:586:GLN:O	1:C:590:THR:CG2	2.63	0.45
1:C:330:MET:HG2	1:C:565:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HG21	1:B:229:HIS:HD2	1.81	0.45
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.52	0.45
1:A:213:LEU:O	1:A:216:VAL:HG22	2.17	0.45
1:D:528:THR:HG22	1:D:554:VAL:HB	1.98	0.45
1:C:388:SER:HB3	1:C:392:ARG:NH1	2.32	0.45
1:C:334:ALA:CB	1:C:568:LEU:HD13	2.47	0.44
1:B:440:PRO:HA	1:B:441:PRO:HD3	1.90	0.44
4:C:805:PEG:H31	1:D:379:GLU:HG2	2.00	0.44
1:B:170:TRP:HB2	1:B:233:ILE:HG22	1.98	0.44
1:C:557:ARG:HD3	1:C:558:PHE:CE2	2.52	0.44
1:D:34:ILE:HD12	1:D:600:LYS:HA	2.00	0.44
1:B:119:LYS:NZ	1:B:138:ASN:OD1	2.50	0.44
1:C:264:ASP:CG	1:C:616:ARG:HH12	2.20	0.44
1:C:357:MET:O	1:C:478:PRO:HA	2.18	0.44
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.53	0.44
1:B:302:HIS:HB2	1:B:432:LEU:HD22	2.00	0.44
1:B:304:CYS:SG	1:B:440:PRO:HD3	2.58	0.44
1:D:14:ALA:HB2	1:D:168:HIS:HB2	2.00	0.43
1:A:517:GLU:O	1:A:521:MET:HG2	2.17	0.43
1:A:271:LEU:HD13	1:A:520:VAL:HG21	2.01	0.43
1:A:450:ASP:OD1	1:A:460:ARG:NH2	2.50	0.43
1:C:295:ASP:HB3	1:C:376:ARG:HH22	1.83	0.43
1:C:123:TRP:O	1:C:127:GLY:HA2	2.18	0.43
1:B:418:LYS:O	1:B:421:ASP:HB2	2.18	0.43
1:A:283:GLN:CG	1:D:280:HIS:CE1	2.99	0.43
1:C:179:CYS:HA	1:C:184:ILE:HD12	2.00	0.43
1:C:549:TYR:O	1:C:590:THR:HB	2.19	0.43
1:D:330:MET:HG2	1:D:565:VAL:HG22	2.01	0.43
1:C:299:GLY:HA2	1:C:375:VAL:HG21	2.00	0.43
1:A:15:THR:HA	1:A:48:PRO:HD2	2.00	0.43
1:B:79:ALA:O	1:B:83:MET:HG2	2.19	0.43
1:A:587:ARG:HA	1:A:590:THR:HG23	2.01	0.43
1:D:350:THR:OG1	1:D:471:ARG:NH1	2.51	0.43
1:A:445:HIS:NE2	1:A:479:GLU:OE1	2.46	0.43
1:C:71:ASP:HA	1:C:74:ARG:HG2	2.01	0.43
1:D:79:ALA:O	1:D:83:MET:HG2	2.19	0.43
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.54	0.42
1:A:3:ARG:NH2	1:A:158:ASP:O	2.51	0.42
1:A:503:VAL:HG21	1:A:572:MET:HE2	2.02	0.42
1:C:323:TYR:OH	1:C:458:LYS:HG3	2.19	0.42
1:C:497:ARG:CZ	1:C:521:MET:HG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LEU:HA	1:C:487:ILE:HD11	2.02	0.42
1:D:463:GLN:HG2	1:D:465:PHE:HE2	1.83	0.42
1:C:137:THR:HG21	1:C:229:HIS:HD2	1.84	0.42
1:D:615:ARG:CZ	1:D:632:ASP:HB3	2.49	0.42
1:D:72:GLU:O	1:D:161:HIS:HE1	2.03	0.42
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.88	0.42
1:A:379:GLU:HG3	1:B:394:PHE:CE1	2.54	0.42
1:C:549:TYR:HB3	1:C:593:LEU:HD11	2.02	0.42
1:C:349:LYS:O	1:C:471:ARG:HG3	2.19	0.42
1:D:484:ASN:O	1:D:485:ASN:C	2.57	0.42
1:C:320:ARG:HH11	2:C:803:UDP:PB	2.43	0.41
1:D:343:LYS:HD3	1:D:469:SER:O	2.20	0.41
1:C:615:ARG:CZ	1:C:632:ASP:HB3	2.50	0.41
1:C:396:HIS:CE1	1:C:405:LEU:HG	2.55	0.41
1:C:565:VAL:O	1:C:569:VAL:HG23	2.20	0.41
1:A:287:ALA:HB2	3:A:802:G6P:H2	2.03	0.41
1:A:510:PRO:O	1:A:532:GLY:HA3	2.20	0.41
1:C:299:GLY:O	1:C:302:HIS:HD2	2.03	0.41
1:D:32:ALA:N	1:D:33:PRO:HD2	2.35	0.41
1:C:79:ALA:O	1:C:83:MET:HG2	2.20	0.41
1:B:25:TYR:CE1	1:B:95:TRP:HZ2	2.39	0.41
1:C:501:LEU:HD21	1:C:526:ILE:HD11	2.02	0.41
1:C:480:PHE:CD1	2:C:803:UDP:C4	3.09	0.41
1:C:296:PHE:CE1	1:C:487:ILE:HG23	2.55	0.41
1:C:94:ARG:HD2	1:C:100:ALA:HB1	2.03	0.41
1:D:369:LEU:HD23	1:D:487:ILE:HD12	2.01	0.41
1:C:323:TYR:OH	1:C:458:LYS:CG	2.69	0.41
1:A:137:THR:HG21	1:A:229:HIS:HD2	1.86	0.41
1:C:250:ILE:CG2	1:C:251:THR:N	2.84	0.40
1:C:74:ARG:NH1	1:C:77:GLN:OE1	2.54	0.40
1:B:24:ILE:CD1	1:B:169:GLN:HG3	2.51	0.40
1:D:192:THR:CG2	1:D:246:THR:HG22	2.52	0.40
1:A:440:PRO:HA	1:A:441:PRO:HD3	1.90	0.40
1:B:278:ALA:HB1	1:B:280:HIS:CE1	2.56	0.40
1:B:234:GLU:HG2	1:B:259:LEU:HD21	2.03	0.40
1:D:17:VAL:HB	1:D:47:GLY:HA3	2.04	0.40
1:C:504:PHE:CD1	1:C:514:THR:CG2	3.05	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)
1:D:85:SER:OG	1:D:85:SER:OG[2_555]	1.92	0.28

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	636/724 (88%)	610 (96%)	24 (4%)	2 (0%)	46 78
1	B	637/724 (88%)	620 (97%)	16 (2%)	1 (0%)	52 84
1	C	636/724 (88%)	611 (96%)	25 (4%)	0	100 100
1	D	631/724 (87%)	600 (95%)	29 (5%)	2 (0%)	46 78
All	All	2540/2896 (88%)	2441 (96%)	94 (4%)	5 (0%)	52 84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLY
1	D	111	VAL
1	D	544	ASN
1	A	111	VAL
1	B	512	GLY

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	553/624 (89%)	523 (95%)	30 (5%)	27 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	554/624 (89%)	519 (94%)	35 (6%)	22 51
1	C	553/624 (89%)	516 (93%)	37 (7%)	20 47
1	D	550/624 (88%)	514 (94%)	36 (6%)	21 49
All	All	2210/2496 (88%)	2072 (94%)	138 (6%)	23 52

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	ASN
1	A	35	THR
1	A	45	LEU
1	A	111	VAL
1	A	135	PHE
1	A	136	GLU
1	A	180	ARG
1	A	181	LYS
1	A	183	ARG
1	A	212	CYS
1	A	227	ILE
1	A	288	LEU
1	A	289	LYS
1	A	310	ASP
1	A	321	TYR
1	A	322	GLU
1	A	376	ARG
1	A	405	LEU
1	A	426	LYS
1	A	458	LYS
1	A	471	ARG
1	A	487	ILE
1	A	531	SER
1	A	537	MET
1	A	541	ILE
1	A	556	ARG
1	A	568	LEU
1	A	590	THR
1	A	634	ASN
1	B	15	THR
1	B	34	ILE
1	B	40	LYS

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	60	ILE
1	B	82	THR
1	B	111	VAL
1	B	123	TRP
1	B	156	HIS
1	B	183	ARG
1	B	199	ARG
1	B	216	VAL
1	B	227	ILE
1	B	249	GLN
1	B	274	ILE
1	B	289	LYS
1	B	291	GLU
1	B	295	ASP
1	B	321	TYR
1	B	348	LYS
1	B	372[A]	GLN
1	B	372[B]	GLN
1	B	376	ARG
1	B	391	LYS
1	B	403	ASN
1	B	428	ARG
1	B	436	GLU
1	B	458	LYS
1	B	531	SER
1	B	537	MET
1	B	543	THR
1	B	545	GLN
1	B	556	ARG
1	B	568	LEU
1	B	590	THR
1	C	15	THR
1	C	82	THR
1	C	111	VAL
1	C	135	PHE
1	C	136	GLU
1	C	181	LYS
1	C	183	ARG
1	C	213	LEU
1	C	220	HIS
1	C	224	ARG

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Mol	Chain	Res	Type
1	C	250	ILE
1	C	275	LYS
1	C	283	GLN
1	C	289	LYS
1	C	320	ARG
1	C	321	TYR
1	C	324	LYS
1	C	347	SER
1	C	363	SER
1	C	376	ARG
1	C	405	LEU
1	C	408	GLU
1	C	417	LEU
1	C	471	ARG
1	C	487	ILE
1	C	537	MET
1	C	539	ASP
1	C	540	LEU
1	C	541	ILE
1	C	542	GLU
1	C	543	THR
1	C	556	ARG
1	C	568	LEU
1	C	590	THR
1	C	595	ASP
1	C	626	VAL
1	C	632	ASP
1	D	12	GLU
1	D	16	GLU
1	D	40	LYS
1	D	45	LEU
1	D	60	ILE
1	D	111	VAL
1	D	115	SER
1	D	135	PHE
1	D	181	LYS
1	D	183	ARG
1	D	213	LEU
1	D	214	GLU
1	D	218	VAL
1	D	249	GLN
1	D	274	ILE

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Mol	Chain	Res	Type
1	D	288	LEU
1	D	289	LYS
1	D	321	TYR
1	D	348	LYS
1	D	372	GLN
1	D	376	ARG
1	D	378	LEU
1	D	405	LEU
1	D	419	SER
1	D	428	ARG
1	D	450	ASP
1	D	487	ILE
1	D	494	GLU
1	D	531	SER
1	D	537	MET
1	D	540	LEU
1	D	556	ARG
1	D	568	LEU
1	D	590	THR
1	D	600	LYS
1	D	611	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	372	GLN
1	A	484	ASN
1	A	582	GLN
1	A	621	GLN
1	A	634	ASN
1	B	7	ASN
1	B	19	ASN
1	B	89	HIS
1	B	582	GLN
1	C	6	GLN
1	C	89	HIS
1	C	249	GLN
1	C	362	ASN
1	C	582	GLN
1	D	8	HIS
1	D	38	GLN
1	D	249	GLN

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Mol	Chain	Res	Type
1	D	582	GLN
1	D	611	GLN
1	D	631	ASN

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

2 carbohydrates 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	$\#\|Z\| > 2$
5	GLC	C	801	-	12,12,12	0.50	0	17,17,17	0.88	0
5	BGC	C	802	-	12,12,12	0.46	0	17,17,17	0.84	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
5	GLC	C	801	-	-	0/2/22/22	0/1/1/1
5	BGC	C	802	-	-	0/2/22/22	0/1/1/1

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.

5.6 Ligand geometry (i)

12 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	UDP	A	801	-	18,26,26	0.81	0	26,40,40	1.55	2 (7%)
3	G6P	A	802	-	16,16,16	0.52	0	23,24,24	0.92	2 (8%)
4	PEG	A	803	-	6,6,6	0.48	0	5,5,5	0.30	0
2	UDP	B	801	-	18,26,26	0.66	0	26,40,40	1.59	3 (11%)
3	G6P	B	802	-	16,16,16	0.49	0	23,24,24	0.77	0
4	PEG	B	803	-	6,6,6	0.44	0	5,5,5	0.43	0
2	UDP	C	803	-	18,26,26	0.86	1 (5%)	26,40,40	1.60	2 (7%)
3	G6P	C	804	-	16,16,16	0.57	0	23,24,24	0.90	2 (8%)
4	PEG	C	805	-	6,6,6	0.39	0	5,5,5	0.41	0
2	UDP	D	801	-	18,26,26	0.77	0	26,40,40	1.70	2 (7%)
3	G6P	D	802	-	16,16,16	0.51	0	23,24,24	1.04	1 (4%)
4	PEG	D	803	-	6,6,6	0.42	0	5,5,5	0.38	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	UDP	A	801	-	-	0/12/32/32	0/2/2/2
3	G6P	A	802	-	-	0/6/26/26	0/1/1/1
4	PEG	A	803	-	-	0/4/4/4	0/0/0/0
2	UDP	B	801	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	B	802	-	-	0/6/26/26	0/1/1/1
4	PEG	B	803	-	-	0/4/4/4	0/0/0/0
2	UDP	C	803	-	-	0/12/32/32	0/2/2/2
3	G6P	C	804	-	-	0/6/26/26	0/1/1/1
4	PEG	C	805	-	-	0/4/4/4	0/0/0/0
2	UDP	D	801	-	-	0/12/32/32	0/2/2/2
3	G6P	D	802	-	-	0/6/26/26	0/1/1/1
4	PEG	D	803	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	803	UDP	O4'-C1'	2.38	1.44	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	UDP	PA-O3A-PB	-3.06	122.40	132.67
2	D	801	UDP	PA-O3A-PB	-3.03	122.51	132.67
2	B	801	UDP	PA-O3A-PB	-2.63	123.86	132.67
3	D	802	G6P	O3-C3-C4	-2.12	105.56	110.34
3	A	802	G6P	O2P-P-O6	-2.10	100.53	106.56
2	B	801	UDP	C4'-O4'-C1'	2.00	111.92	109.72
3	C	804	G6P	C1-O5-C5	2.01	117.19	113.47
3	C	804	G6P	O2P-P-O1P	2.14	115.53	107.38
2	C	803	UDP	O3B-PB-O2B	2.17	115.66	107.38
3	A	802	G6P	O2P-P-O1P	2.41	116.56	107.38
2	A	801	UDP	C4-N3-C2	5.45	119.54	114.14
2	B	801	UDP	C4-N3-C2	5.96	120.04	114.14
2	C	803	UDP	C4-N3-C2	6.00	120.08	114.14
2	D	801	UDP	C4-N3-C2	6.73	120.81	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	G6P	3	0
4	A	803	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	UDP	1	0
3	B	802	G6P	1	0
4	B	803	PEG	1	0
2	C	803	UDP	3	0
4	C	805	PEG	2	0
4	D	803	PEG	1	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

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	638/724 (88%)	0.29	28 (4%)	38	30	41, 61, 110, 139	0
1	B	638/724 (88%)	0.07	15 (2%)	62	55	33, 53, 106, 139	0
1	C	638/724 (88%)	0.25	33 (5%)	31	23	40, 59, 111, 142	1 (0%)
1	D	635/724 (87%)	0.42	53 (8%)	14	8	35, 72, 137, 165	0
All	All	2549/2896 (88%)	0.26	129 (5%)	32	23	33, 59, 123, 165	1 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	630	LEU	7.3
1	D	637	ALA	6.6
1	D	626	VAL	6.2
1	D	627	GLY	5.6
1	D	122	LEU	5.5
1	C	128	ILE	5.5
1	D	622	PHE	5.3
1	D	128	ILE	5.2
1	D	125	LEU	5.2
1	D	629	GLU	5.1
1	D	628	GLU	5.0
1	D	132	GLU	4.6
1	B	624	GLU	4.6
1	A	61	LEU	4.6
1	C	129	PRO	4.3
1	D	126	VAL	4.2
1	D	620	ASP	4.1
1	C	133	ASN	4.1
1	D	123	TRP	4.0
1	D	638	LEU	4.0
1	D	631	ASN	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	135	PHE	4.0
1	A	60	ILE	4.0
1	B	630	LEU	4.0
1	D	133	ASN	4.0
1	D	205	GLY	4.0
1	C	68	ALA	3.9
1	C	125	LEU	3.9
1	A	62	ASP	3.8
1	A	543	THR	3.8
1	D	76	VAL	3.8
1	D	624	GLU	3.7
1	A	92	TYR	3.7
1	D	625	LEU	3.7
1	D	615	ARG	3.6
1	A	76	VAL	3.5
1	B	2	SER	3.5
1	C	116	ASN	3.5
1	D	55	GLN	3.4
1	C	114	TYR	3.4
1	C	123	TRP	3.4
1	C	126	VAL	3.4
1	D	61	LEU	3.4
1	A	69	PHE	3.4
1	C	549	TYR	3.4
1	A	157	LEU	3.3
1	D	124	SER	3.3
1	D	70	SER	3.3
1	D	59	ASP	3.2
1	D	614	LEU	3.2
1	A	63	TRP	3.2
1	C	124	SER	3.0
1	C	88	VAL	2.9
1	C	436	GLU	2.9
1	C	60	ILE	2.9
1	C	111	VAL	2.9
1	B	65	LYS	2.9
1	D	94	ARG	2.8
1	D	639	ALA	2.8
1	C	118	TRP	2.8
1	A	104	ILE	2.8
1	C	62	ASP	2.8
1	A	64	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	2	SER	2.8
1	A	88	VAL	2.7
1	B	71	ASP	2.7
1	B	622	PHE	2.7
1	A	448	VAL	2.7
1	A	90	PHE	2.7
1	B	637	ALA	2.7
1	A	77	GLN	2.7
1	D	623	ARG	2.7
1	B	67	GLU	2.7
1	A	68	ALA	2.7
1	A	58	VAL	2.6
1	C	131	PRO	2.6
1	A	544	ASN	2.6
1	D	136	GLU	2.6
1	A	66	PRO	2.6
1	B	629	GLU	2.5
1	C	127	GLY	2.5
1	D	117	GLU	2.5
1	A	406	THR	2.5
1	C	113	GLY	2.5
1	D	632	ASP	2.5
1	B	61	LEU	2.5
1	A	82	THR	2.4
1	D	5	LEU	2.4
1	A	156	HIS	2.4
1	A	59	ASP	2.4
1	C	544	ASN	2.4
1	D	127	GLY	2.4
1	D	63	TRP	2.4
1	D	112	ARG	2.4
1	D	115	SER	2.4
1	D	99	GLY	2.4
1	A	49	LEU	2.3
1	B	132	GLU	2.3
1	C	545	GLN	2.3
1	A	67	GLU	2.3
1	C	592	ARG	2.3
1	A	153	GLU	2.2
1	B	5	LEU	2.2
1	C	112	ARG	2.2
1	C	229	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	67	GLU	2.2
1	D	224	ARG	2.2
1	C	67	GLU	2.2
1	C	220	HIS	2.2
1	D	636	ASP	2.2
1	C	122	LEU	2.2
1	D	242	ASP	2.2
1	D	66	PRO	2.1
1	B	78	HIS	2.1
1	A	203	ALA	2.1
1	D	228	TYR	2.1
1	C	593	LEU	2.1
1	B	74	ARG	2.1
1	D	265	GLY	2.1
1	B	64	LYS	2.1
1	C	437	GLY	2.1
1	C	624	GLU	2.1
1	D	604	LEU	2.1
1	A	78	HIS	2.1
1	D	96	LEU	2.0
1	C	83	MET	2.0
1	D	611	GLN	2.0
1	D	225	PHE	2.0
1	D	62	ASP	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)

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, 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	LLDF	B-factors(Å^2)	Q<0.9
5	BGC	C	802	12/12	0.98	0.16	-0.25	53,57,59,60	12
5	GLC	C	801	12/12	0.98	0.15	-0.86	46,49,51,53	12

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	PEG	B	803	7/7	0.91	0.26	2.73	68,69,76,76	0
4	PEG	D	803	7/7	0.92	0.21	1.76	55,65,75,78	0
2	UDP	C	803	25/25	0.97	0.19	0.26	39,51,55,59	0
3	G6P	B	802	16/16	0.98	0.17	0.01	36,41,45,47	0
4	PEG	A	803	7/7	0.86	0.18	-0.03	73,77,85,85	0
3	G6P	A	802	16/16	0.99	0.17	-0.39	42,48,52,52	0
3	G6P	D	802	16/16	0.99	0.16	-0.54	35,40,44,46	0
3	G6P	C	804	16/16	0.98	0.15	-1.05	43,47,49,52	0
2	UDP	B	801	25/25	0.97	0.15	-1.28	46,57,85,89	0
2	UDP	A	801	25/25	0.97	0.14	-1.40	47,59,72,73	0
2	UDP	D	801	25/25	0.98	0.12	-1.84	48,58,70,71	0
4	PEG	C	805	7/7	0.94	0.13	-1.91	62,69,77,78	0

6.5 Other polymers

There are no such residues in this entry.