



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2017 – 07:40 AM EDT

PDB ID : 5T0A
Title : Crystal Structure of Heparan Sulfate 6-O-Sulfotransferase with bound PAP and heptasaccharide substrate
Authors : Pedersen, L.C.; Moon, A.F.; Krahn, J.M.; Liu, J.
Deposited on : unknown
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029824

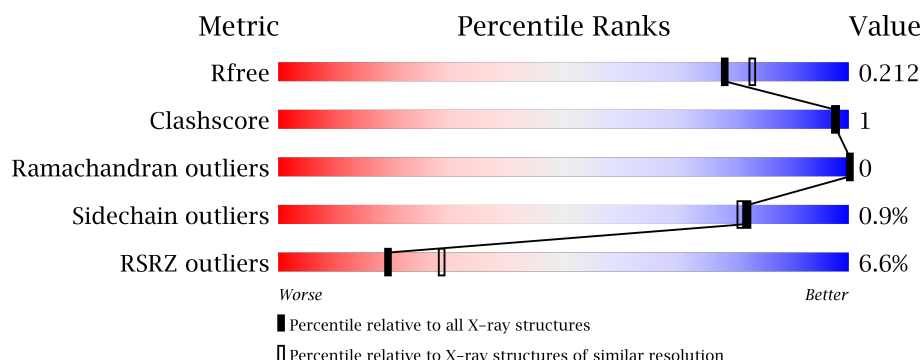
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	692	<div> <div>5%</div> <div>95%</div> <div>..</div> </div>
1	B	692	<div> <div>8%</div> <div>95%</div> <div>..</div> </div>

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
3	BDP	B	1401	-	-	-	X
5	NPO	A	2007	-	-	-	X
6	GLC	A	2008	-	-	-	X
8	EDO	A	2015	-	-	-	X
8	EDO	A	2020	-	-	-	X
8	EDO	B	1417	-	-	-	X
9	TLA	A	2024	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 12008 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 maltose binding protein - heparan sulfate 6-O-sulfotransferase isoform 3 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	3	0
			5234	3337	890	981	26			
1	B	677	Total	C	N	O	S	0	7	0
			5296	3376	896	997	27			

There are 26 discrepancies between the modelled and reference sequences:

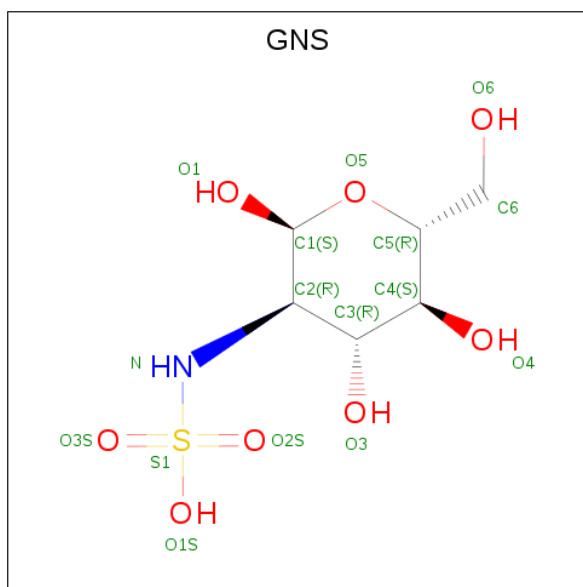
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0AEY0
A	82	ALA	ASP	engineered mutation	UNP P0AEY0
A	83	ALA	LYS	engineered mutation	UNP P0AEY0
A	172	ALA	GLU	engineered mutation	UNP P0AEY0
A	173	ALA	ASN	engineered mutation	UNP P0AEY0
A	239	ALA	LYS	engineered mutation	UNP P0AEY0
A	359	ALA	GLU	engineered mutation	UNP P0AEY0
A	362	ALA	LYS	engineered mutation	UNP P0AEY0
A	363	ALA	ASP	engineered mutation	UNP P0AEY0
A	367	ASN	-	linker	UNP P0AEY0
A	368	ALA	-	linker	UNP P0AEY0
A	369	ALA	-	linker	UNP P0AEY0
A	370	ALA	-	linker	UNP P0AEY0
B	0	MET	-	initiating methionine	UNP P0AEY0
B	82	ALA	ASP	engineered mutation	UNP P0AEY0
B	83	ALA	LYS	engineered mutation	UNP P0AEY0
B	172	ALA	GLU	engineered mutation	UNP P0AEY0
B	173	ALA	ASN	engineered mutation	UNP P0AEY0
B	239	ALA	LYS	engineered mutation	UNP P0AEY0
B	359	ALA	GLU	engineered mutation	UNP P0AEY0
B	362	ALA	LYS	engineered mutation	UNP P0AEY0
B	363	ALA	ASP	engineered mutation	UNP P0AEY0
B	367	ASN	-	linker	UNP P0AEY0
B	368	ALA	-	linker	UNP P0AEY0

Continued on next page...

Continued from previous page...

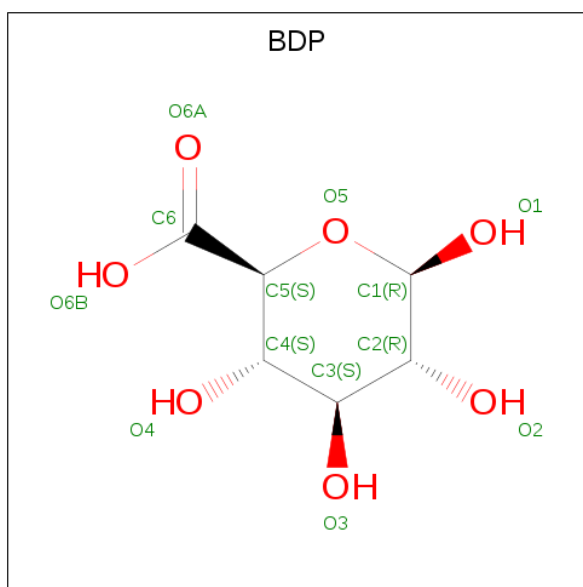
Chain	Residue	Modelled	Actual	Comment	Reference
B	369	ALA	-	linker	UNP P0AEY0
B	370	ALA	-	linker	UNP P0AEY0

- Molecule 2 is N-SULFO-ALPHA-D-GLUCOSAMINE (three-letter code: GNS) (formula: $C_6H_{13}NO_8S$).



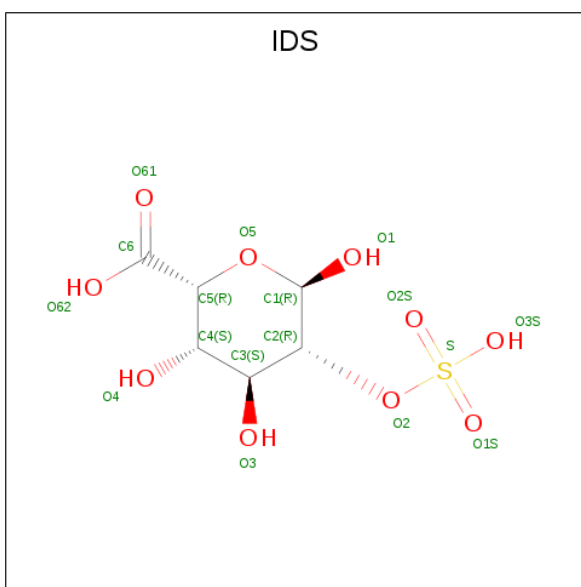
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	6	1	7	1		
2	A	1	Total	C	N	O	S	0	0
			15	6	1	7	1		
2	A	1	Total	C	N	O	S	0	0
			15	6	1	7	1		
2	B	1	Total	C	N	O	S	0	0
			15	6	1	7	1		
2	B	1	Total	C	N	O	S	0	1
			30	12	2	14	2		
2	B	1	Total	C	N	O	S	0	1
			15	6	1	7	1		

- Molecule 3 is BETA-D-GLUCOPYRANURONIC ACID (three-letter code: BDP) (formula: $C_6H_{10}O_7$).



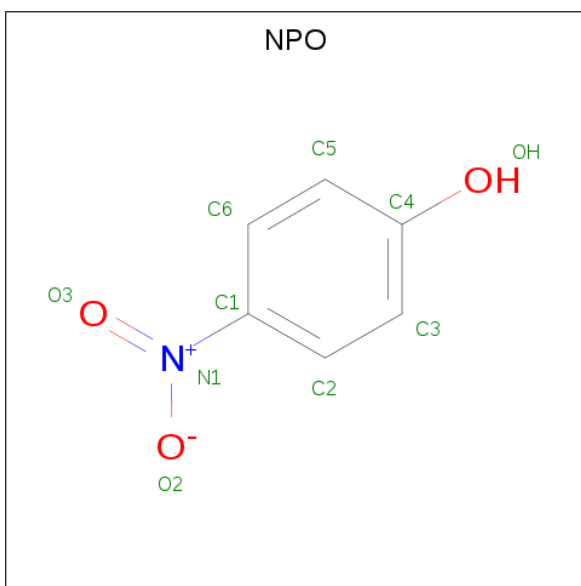
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 4 is 2-O-sulfo-alpha-L-idopyranuronic acid (three-letter code: IDS) (formula: $C_6H_{10}O_{10}S$).



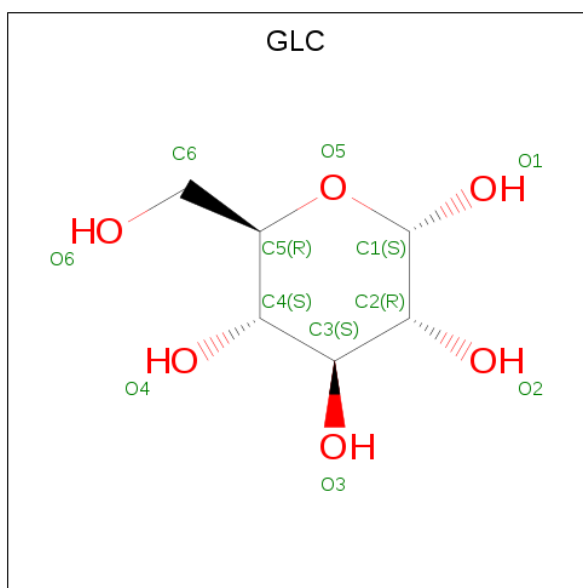
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			16	6	9	1		
4	B	1	Total	C	O	S	0	1
			16	6	9	1		

- Molecule 5 is P-NITROPHENOL (three-letter code: NPO) (formula: $C_6H_5NO_3$).



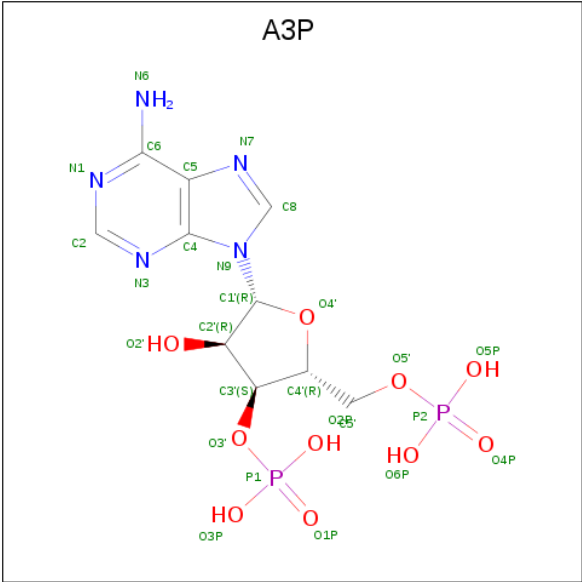
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			10	6	1	3		
5	B	1	Total	C	O		0	1
			7	6	1			

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



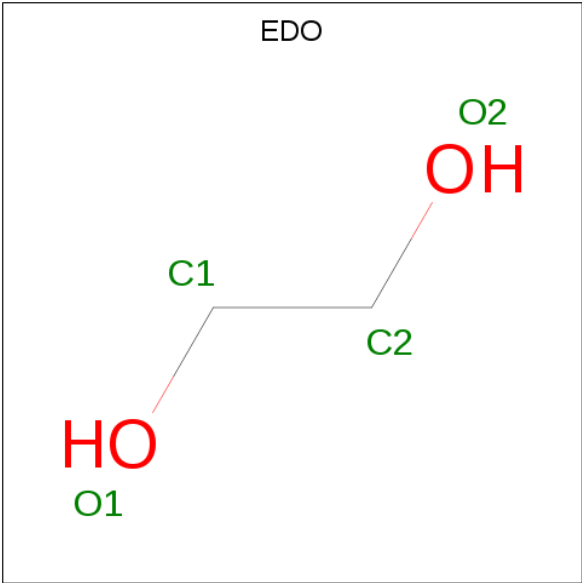
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			12	6	6		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			11	6	5		
6	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is ADENOSINE-3'-5'-DIPHOSPHATE (three-letter code: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



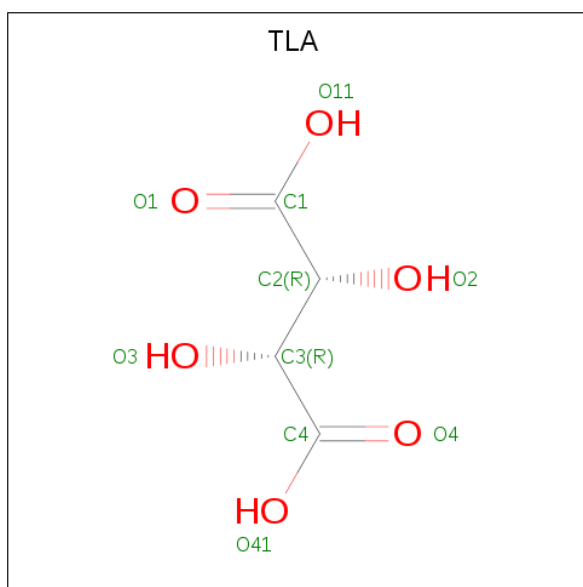
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 8	C 4	O 4	0	1
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	A	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0
8	B	1	Total 4	C 2	O 2	0	0

- Molecule 9 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	4	6		
9	A	1	Total	C	O	0	0
			10	4	6		
9	B	1	Total	C	O	0	0
			10	4	6		

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	2	Total	Na	0	0
			2	2		
10	A	4	Total	Na	0	0
			4	4		

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Cl	0	0
			1	1		
11	A	2	Total	Cl	0	0
			2	2		

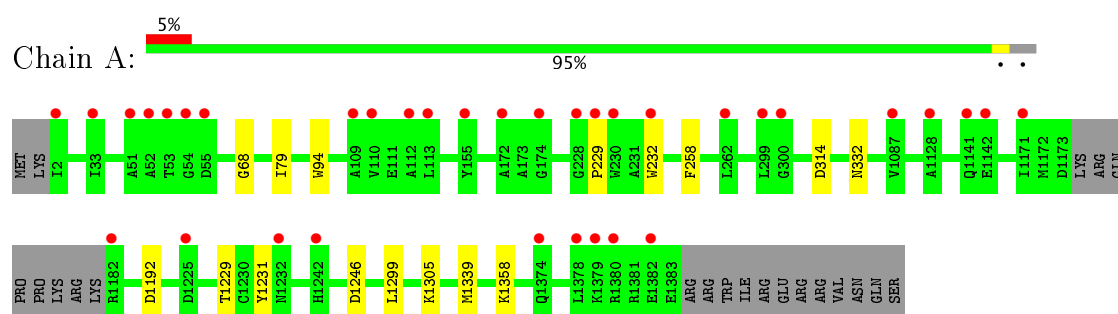
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	524	Total 527	O 527	0	3
12	B	487	Total 490	O 490	0	3

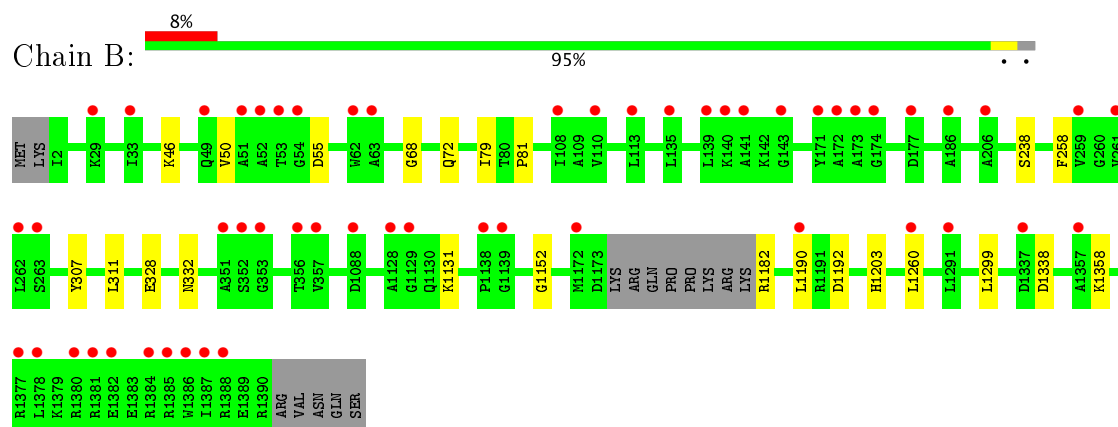
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: maltose binding protein - heparan sulfate 6-O-sulfotransferase isoform 3 fusion protein



- Molecule 1: maltose binding protein - heparan sulfate 6-O-sulfotransferase isoform 3 fusion protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.78Å 128.29Å 178.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.84 – 1.95 37.89 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.84-1.95) 95.5 (37.89-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.180 , 0.213 0.177 , 0.212	Depositor DCC
R_{free} test set	2703 reflections (2.22%)	DCC
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12008	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNS, NPO, A3P, CL, NA, GLC, IDS, EDO, TLA, BDP

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	0/5357	0.55	0/7275
1	B	0.41	0/5421	0.54	0/7367
All	All	0.40	0/10778	0.54	0/14642

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	5234	0	5013	7	0
1	B	5296	0	5029	12	0
2	A	45	0	28	1	0
2	B	60	0	36	0	0
3	A	24	0	12	0	0
3	B	36	0	19	1	0
4	A	16	0	6	0	0
4	B	16	0	5	0	0
5	A	10	0	4	0	0
5	B	7	0	4	0	0
6	A	45	0	39	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	45	0	39	0	0
7	A	27	0	11	0	0
7	B	27	0	11	0	0
8	A	48	0	72	0	0
8	B	16	0	24	0	0
9	A	20	0	8	1	0
9	B	10	0	4	0	0
10	A	4	0	0	0	0
10	B	2	0	0	0	0
11	A	2	0	0	1	0
11	B	1	0	0	0	0
12	A	527	0	0	2	0
12	B	490	0	0	4	0
All	All	12008	0	10364	20	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 1.

All (20) 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:1131[A]:LYS:NZ	12:B:1505:HOH:O	2.32	0.60
1:B:72[B]:GLN:NE2	12:B:1509:HOH:O	2.35	0.60
11:A:2031:CL:CL	12:A:2534:HOH:O	2.54	0.58
1:B:307:TYR:CE2	1:B:311:LEU:HD11	2.44	0.51
1:B:68:GLY:HA3	1:B:332:ASN:O	2.11	0.51
1:B:46:LYS:O	1:B:50:VAL:HG22	2.10	0.51
1:A:1299:LEU:HD11	1:A:1358:LYS:HA	1.93	0.50
1:A:314:ASP:OD2	12:A:2101:HOH:O	2.19	0.47
1:B:79:ILE:HG22	1:B:81:PRO:HD3	1.96	0.47
1:B:1299:LEU:HD11	1:B:1358:LYS:HA	1.96	0.46
1:B:1182:ARG:NH2	12:B:1512:HOH:O	2.43	0.45
1:A:68:GLY:HA3	1:A:332:ASN:O	2.17	0.44
1:A:1305:LYS:NZ	1:B:238:SER:O	2.46	0.44
1:B:1152:GLY:O	12:B:1503:HOH:O	2.21	0.44
1:A:229:PRO:HA	1:A:232:TRP:CE2	2.54	0.43
1:B:1203:HIS:CE1	3:B:1401:BDP:H5	2.54	0.42
2:A:2001:GNS:O4	9:A:2025:TLA:H3	2.19	0.42
1:B:1190[A]:LEU:HD21	1:B:1260:LEU:HD11	2.01	0.41
1:A:1229:THR:HG22	1:A:1231:TYR:H	1.85	0.41
1:A:79:ILE:HD11	1:A:94:TRP:HZ3	1.85	0.41

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	669/692 (97%)	657 (98%)	12 (2%)	0	100	100
1	B	679/692 (98%)	667 (98%)	12 (2%)	0	100	100
All	All	1348/1384 (97%)	1324 (98%)	24 (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	531/582 (91%)	527 (99%)	4 (1%)	85	83
1	B	534/582 (92%)	529 (99%)	5 (1%)	82	81
All	All	1065/1164 (92%)	1056 (99%)	9 (1%)	82	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	PHE
1	A	1192	ASP
1	A	1246	ASP
1	A	1339	MET
1	B	55	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	258	PHE
1	B	328	GLU
1	B	1192	ASP
1	B	1338	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1275	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 54 ligands modelled in this entry, 9 are monoatomic - leaving 45 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	GNS	A	2001	3	14,15,16	0.94	1 (7%)	15,22,24	1.64	3 (20%)
3	BDP	A	2002	10,2	9,12,13	0.81	0	13,17,19	1.05	1 (7%)
2	GNS	A	2003	10,3,4	14,15,16	0.67	1 (7%)	15,22,24	1.09	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IDS	A	2004	10,2	13,16,17	0.79	0	15,24,26	0.84	1 (6%)
2	GNS	A	2005	3,4	14,15,16	0.69	0	15,22,24	1.10	1 (6%)
3	BDP	A	2006	2,5	9,12,13	0.90	0	13,17,19	0.90	1 (7%)
5	NPO	A	2007	3	9,10,10	1.03	0	11,13,13	0.73	0
6	GLC	A	2008	6	11,11,12	0.60	0	13,15,17	1.71	1 (7%)
6	GLC	A	2009	6	11,11,12	0.90	1 (9%)	13,15,17	0.92	0
6	GLC	A	2010	6	11,11,12	0.62	0	13,15,17	1.11	1 (7%)
6	GLC	A	2011	6	12,12,12	0.36	0	17,17,17	1.00	0
7	A3P	A	2012	-	26,29,29	0.67	0	31,45,45	0.76	1 (3%)
8	EDO	A	2013	-	3,3,3	0.43	0	2,2,2	0.35	0
8	EDO	A	2014	-	3,3,3	0.42	0	2,2,2	0.30	0
8	EDO	A	2015	-	3,3,3	0.55	0	2,2,2	0.50	0
8	EDO	A	2016	-	3,3,3	0.32	0	2,2,2	0.68	0
8	EDO	A	2017	-	3,3,3	0.43	0	2,2,2	0.47	0
8	EDO	A	2018	-	3,3,3	0.45	0	2,2,2	0.35	0
8	EDO	A	2019[A]	-	3,3,3	0.45	0	2,2,2	0.38	0
8	EDO	A	2019[B]	-	3,3,3	0.45	0	2,2,2	0.45	0
8	EDO	A	2020	-	3,3,3	0.41	0	2,2,2	0.23	0
8	EDO	A	2021	-	3,3,3	0.28	0	2,2,2	0.70	0
8	EDO	A	2022	-	3,3,3	0.43	0	2,2,2	0.30	0
8	EDO	A	2023	-	3,3,3	0.44	0	2,2,2	0.34	0
9	TLA	A	2024	-	3,9,9	0.47	0	6,12,12	1.39	1 (16%)
9	TLA	A	2025	10	3,9,9	0.47	0	6,12,12	1.49	1 (16%)
3	BDP	B	1401	2	9,12,13	1.00	1 (11%)	13,17,19	1.83	3 (23%)
2	GNS	B	1402	3	14,15,16	0.79	0	15,22,24	2.18	4 (26%)
3	BDP	B	1403	2	9,12,13	1.06	1 (11%)	13,17,19	1.48	2 (15%)
2	GNS	B	1404[A]	3,4	14,15,16	0.90	0	15,22,24	2.00	6 (40%)
2	GNS	B	1404[B]	3	14,15,16	0.54	0	15,22,24	1.64	4 (26%)
4	IDS	B	1405[A]	2	13,16,17	0.84	0	15,24,26	1.15	1 (6%)
2	GNS	B	1406[A]	3,4	14,15,16	0.73	0	15,22,24	1.60	3 (20%)
3	BDP	B	1407[A]	2,5	9,12,13	0.91	0	13,17,19	1.41	1 (7%)
5	NPO	B	1408[A]	3	7,7,10	1.03	1 (14%)	8,8,13	0.83	0
6	GLC	B	1409	6	11,11,12	0.67	0	13,15,17	1.52	3 (23%)
6	GLC	B	1410	6	11,11,12	0.64	0	13,15,17	0.98	0
6	GLC	B	1411	6	11,11,12	0.62	0	13,15,17	1.12	1 (7%)
6	GLC	B	1412	6	12,12,12	0.54	0	17,17,17	0.67	0
7	A3P	B	1413	-	26,29,29	0.66	0	31,45,45	0.82	0
8	EDO	B	1414	-	3,3,3	0.60	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	B	1415	-	3,3,3	0.46	0	2,2,2	0.54	0
8	EDO	B	1416	-	3,3,3	0.30	0	2,2,2	0.72	0
8	EDO	B	1417	-	3,3,3	0.48	0	2,2,2	0.46	0
9	TLA	B	1418	-	3,9,9	0.08	0	6,12,12	1.00	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	GNS	A	2001	3	-	0/6/24/27	0/1/1/1
3	BDP	A	2002	10,2	-	0/0/21/24	0/1/1/1
2	GNS	A	2003	10,3,4	-	0/6/24/27	0/1/1/1
4	IDS	A	2004	10,2	-	0/5/26/29	0/1/1/1
2	GNS	A	2005	3,4	-	0/6/24/27	0/1/1/1
3	BDP	A	2006	2,5	-	0/0/21/24	0/1/1/1
5	NPO	A	2007	3	-	0/2/4/4	0/1/1/1
6	GLC	A	2008	6	-	0/2/19/22	0/1/1/1
6	GLC	A	2009	6	-	0/2/19/22	0/1/1/1
6	GLC	A	2010	6	-	0/2/19/22	0/1/1/1
6	GLC	A	2011	6	-	0/2/22/22	0/1/1/1
7	A3P	A	2012	-	-	0/11/31/31	0/3/3/3
8	EDO	A	2013	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2014	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2015	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2016	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2017	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2018	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2019[A]	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2019[B]	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2020	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2021	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2022	-	-	0/1/1/1	0/0/0/0
8	EDO	A	2023	-	-	0/1/1/1	0/0/0/0
9	TLA	A	2024	-	-	0/4/12/12	0/0/0/0
9	TLA	A	2025	10	-	0/4/12/12	0/0/0/0
3	BDP	B	1401	2	-	0/0/21/24	0/1/1/1
2	GNS	B	1402	3	-	0/6/24/27	0/1/1/1
3	BDP	B	1403	2	-	0/0/21/24	0/1/1/1
2	GNS	B	1404[A]	3,4	-	0/6/24/27	0/1/1/1
2	GNS	B	1404[B]	3	-	0/6/24/27	0/1/1/1
4	IDS	B	1405[A]	2	-	0/5/26/29	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNS	B	1406[A]	3,4	-	0/6/24/27	0/1/1/1
3	BDP	B	1407[A]	2,5	-	0/0/21/24	0/1/1/1
5	NPO	B	1408[A]	3	-	0/0/0/4	0/1/1/1
6	GLC	B	1409	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1410	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1411	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1412	6	-	0/2/22/22	0/1/1/1
7	A3P	B	1413	-	-	0/11/31/31	0/3/3/3
8	EDO	B	1414	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1415	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1416	-	-	0/1/1/1	0/0/0/0
8	EDO	B	1417	-	-	0/1/1/1	0/0/0/0
9	TLA	B	1418	-	-	0/4/12/12	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1403	BDP	O5-C5	-2.35	1.41	1.43
6	A	2009	GLC	O5-C1	-2.31	1.39	1.43
3	B	1401	BDP	O5-C5	-2.11	1.41	1.43
2	A	2003	GNS	S1-N	2.02	1.62	1.59
2	A	2001	GNS	S1-N	2.08	1.62	1.59
5	B	1408[A]	NPO	OH-C4	2.13	1.42	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1402	GNS	O3S-S1-O2S	-4.80	107.44	120.23
2	B	1404[B]	GNS	O3S-S1-O2S	-4.17	109.10	120.23
2	B	1404[A]	GNS	O5-C1-C2	-3.85	106.11	111.47
3	B	1403	BDP	O5-C1-C2	-3.77	104.88	110.79
2	B	1406[A]	GNS	O3S-S1-O2S	-3.51	110.88	120.23
2	A	2001	GNS	O3S-S1-O2S	-3.49	110.92	120.23
2	B	1404[A]	GNS	C3-C4-C5	-3.33	104.35	110.22
9	A	2025	TLA	C4-C3-C2	-3.32	105.95	113.11
3	B	1401	BDP	O5-C1-C2	-3.32	105.59	110.79
2	B	1402	GNS	O5-C1-C2	-3.08	107.19	111.47
2	B	1406[A]	GNS	O5-C1-C2	-3.06	107.22	111.47
9	A	2024	TLA	C1-C2-C3	-2.99	106.68	113.11
6	B	1411	GLC	C1-C2-C3	-2.78	106.13	109.65
2	A	2005	GNS	O3S-S1-O2S	-2.76	112.87	120.23
2	B	1404[B]	GNS	O5-C1-C2	-2.72	107.68	111.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1404[A]	GNS	O3S-S1-O2S	-2.71	113.00	120.23
6	B	1409	GLC	C2-C3-C4	-2.55	106.43	110.88
2	A	2003	GNS	O5-C1-C2	-2.52	107.97	111.47
2	B	1404[A]	GNS	C4-C3-C2	-2.43	107.45	111.02
2	B	1404[A]	GNS	C1-C2-N	-2.43	106.02	110.29
3	B	1403	BDP	O2-C2-C3	-2.36	105.54	110.17
2	A	2001	GNS	O5-C1-C2	-2.21	108.40	111.47
6	A	2010	GLC	O5-C1-C2	-2.18	107.37	110.79
6	B	1409	GLC	O2-C2-C3	-2.15	105.95	110.17
2	B	1404[B]	GNS	C6-C5-C4	-2.12	108.04	113.00
2	B	1404[B]	GNS	C3-C4-C5	2.00	113.75	110.22
7	A	2012	A3P	O6P-P2-O4P	2.10	118.72	110.50
2	B	1404[A]	GNS	O3-C3-C4	2.29	115.35	110.36
4	A	2004	IDS	C1-C2-C3	2.38	112.97	109.40
3	A	2002	BDP	O5-C5-C4	2.49	113.10	108.93
3	A	2006	BDP	C1-C2-C3	2.64	113.00	109.65
6	B	1409	GLC	C1-O5-C5	2.70	115.89	112.17
2	B	1406[A]	GNS	C1-O5-C5	3.07	116.40	112.17
4	B	1405[A]	IDS	C1-C2-C3	3.12	114.09	109.40
3	B	1401	BDP	O5-C5-C4	3.19	114.28	108.93
3	B	1401	BDP	O2-C2-C1	3.25	115.78	109.18
2	A	2001	GNS	C1-O5-C5	3.67	117.22	112.17
3	B	1407[A]	BDP	C1-C2-C3	3.79	114.46	109.65
2	B	1402	GNS	C1-O5-C5	4.11	117.83	112.17
2	B	1402	GNS	O2S-S1-N	4.11	113.90	108.49
6	A	2008	GLC	C1-O5-C5	5.17	119.30	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	GNS	1	0
9	A	2025	TLA	1	0
3	B	1401	BDP	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	670/692 (96%)	0.19	35 (5%)	28 38	17, 32, 55, 83	0
1	B	677/692 (97%)	0.41	54 (7%)	13 21	15, 35, 55, 75	11 (1%)
All	All	1347/1384 (97%)	0.30	89 (6%)	19 28	15, 33, 55, 83	11 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	ALA	7.5
1	B	1386	TRP	7.3
1	B	1387	ILE	5.2
1	B	141	ALA	5.1
1	A	52	ALA	5.1
1	B	52	ALA	4.3
1	B	186	ALA	4.2
1	A	230	TRP	3.9
1	B	172	ALA	3.9
1	B	139	LEU	3.9
1	B	1378	LEU	3.8
1	B	171	TYR	3.7
1	B	1139	GLY	3.7
1	B	1385	ARG	3.4
1	A	113	LEU	3.4
1	B	135	LEU	3.4
1	A	51	ALA	3.4
1	A	1379	LYS	3.3
1	B	351	ALA	3.3
1	B	174	GLY	3.2
1	B	353	GLY	3.2
1	A	1378	LEU	3.2
1	A	33	ILE	3.2
1	A	2	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1088	ASP	3.0
1	A	299	LEU	2.9
1	A	174	GLY	2.9
1	B	62	TRP	2.9
1	B	1388	ARG	2.9
1	A	53	THR	2.8
1	B	33	ILE	2.8
1	B	1337	ASP	2.8
1	B	1377	ARG	2.7
1	B	262	LEU	2.7
1	A	54	GLY	2.6
1	B	1128	ALA	2.6
1	B	1129	GLY	2.6
1	A	1141	GLN	2.6
1	A	1232	ASN	2.5
1	A	1225	ASP	2.5
1	B	53	THR	2.5
1	B	357	VAL	2.5
1	A	112	ALA	2.5
1	A	1374	GLN	2.5
1	B	1291	LEU	2.5
1	A	1128	ALA	2.4
1	B	143	GLY	2.4
1	A	155	TYR	2.4
1	B	113	LEU	2.4
1	A	109	ALA	2.4
1	B	1190[A]	LEU	2.4
1	B	49	GLN	2.4
1	A	1087	VAL	2.3
1	A	262	LEU	2.3
1	B	1260	LEU	2.3
1	B	259	VAL	2.3
1	A	55	ASP	2.3
1	A	1142	GLU	2.2
1	B	1382	GLU	2.2
1	B	29	LYS	2.2
1	B	356	THR	2.2
1	A	110	VAL	2.2
1	A	228	GLY	2.2
1	B	1380	ARG	2.2
1	B	108	ILE	2.2
1	A	232	TRP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1357	ALA	2.2
1	A	1380	ARG	2.1
1	B	206	ALA	2.1
1	B	110	VAL	2.1
1	B	263	SER	2.1
1	B	1384	ARG	2.1
1	B	54	GLY	2.1
1	A	1242	HIS	2.1
1	A	1171	ILE	2.1
1	B	51	ALA	2.1
1	A	229	PRO	2.1
1	B	1138	PRO	2.1
1	B	177	ASP	2.1
1	A	1382	GLU	2.1
1	A	300	GLY	2.1
1	A	1182	ARG	2.0
1	B	1172	MET	2.0
1	A	172	ALA	2.0
1	B	140	LYS	2.0
1	B	352	SER	2.0
1	B	261	VAL	2.0
1	B	1381	ARG	2.0
1	B	63	ALA	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(\AA^2)	Q<0.9
5	NPO	A	2007	10/10	0.94	0.25	7.17	36,46,53,56	0
8	EDO	A	2020	4/4	0.92	0.18	3.83	31,40,45,49	4
6	GLC	A	2008	11/12	0.83	0.20	3.79	29,37,41,42	11
8	EDO	A	2015	4/4	0.83	0.17	3.78	27,27,28,41	0
8	EDO	B	1417	4/4	0.89	0.24	3.62	34,37,42,44	4
3	BDP	B	1401	12/13	0.83	0.19	3.04	29,35,41,50	12
9	TLA	A	2024	10/10	0.88	0.25	2.16	42,49,51,58	10
8	EDO	A	2022	4/4	0.92	0.15	1.74	28,36,41,43	4
8	EDO	A	2018	4/4	0.90	0.14	1.42	34,34,39,44	0
6	GLC	B	1409	11/12	0.85	0.16	1.30	36,49,53,55	11
6	GLC	A	2011	12/12	0.98	0.22	0.99	23,24,27,29	0
6	GLC	A	2010	11/12	0.97	0.17	0.85	18,23,24,25	0
8	EDO	A	2017	4/4	0.93	0.16	0.74	34,35,38,46	0
8	EDO	A	2021	4/4	0.88	0.15	0.69	31,37,40,47	4
2	GNS	B	1404[A]	15/16	0.92	0.13	0.54	34,37,44,49	15
8	EDO	B	1414	4/4	0.90	0.13	0.51	24,25,26,32	0
10	NA	B	1419	1/1	0.97	0.11	0.48	37,37,37,37	1
8	EDO	B	1415	4/4	0.91	0.14	0.41	31,31,33,42	4
8	EDO	A	2013	4/4	0.94	0.11	0.41	32,36,39,42	0
8	EDO	B	1416	4/4	0.98	0.12	0.27	19,23,24,30	4
7	A3P	A	2012	27/27	0.98	0.12	0.19	19,22,24,26	0
11	CL	B	1421	1/1	0.96	0.12	0.09	37,37,37,37	1
2	GNS	B	1402	15/16	0.99	0.10	-0.06	19,24,28,32	0
6	GLC	B	1411	11/12	0.96	0.15	-0.16	26,28,31,32	0
6	GLC	B	1412	12/12	0.96	0.17	-0.29	27,29,34,34	0
7	A3P	B	1413	27/27	0.98	0.11	-0.30	18,20,23,24	0
8	EDO	A	2014	4/4	0.94	0.09	-0.60	37,37,42,46	0
10	NA	A	2027	1/1	0.96	0.08	-0.73	41,41,41,41	0
2	GNS	A	2001	15/16	0.98	0.08	-0.76	25,28,33,36	0
6	GLC	B	1410	11/12	0.94	0.10	-0.78	33,36,39,39	0
11	CL	A	2030	1/1	0.99	0.06	-1.73	27,27,27,27	0
6	GLC	A	2009	11/12	0.98	0.08	-1.81	23,28,31,32	0
8	EDO	A	2016	4/4	0.98	0.07	-2.68	30,32,32,36	0
4	IDS	A	2004	16/17	0.94	0.16	-	39,45,52,55	0
3	BDP	A	2006	12/13	0.92	0.18	-	45,49,56,58	0
4	IDS	B	1405[A]	16/17	0.94	0.08	-	39,42,49,51	16
9	TLA	A	2025	10/10	0.84	0.23	-	36,38,48,48	10
10	NA	A	2029	1/1	0.80	0.19	-	55,55,55,55	0
3	BDP	B	1403	12/13	0.96	0.09	-	22,25,31,33	0
9	TLA	B	1418	10/10	0.92	0.16	-	25,30,37,38	10
3	BDP	B	1407[A]	12/13	0.86	0.12	-	55,57,64,66	12
11	CL	A	2031	1/1	0.96	0.06	-	40,40,40,40	1
3	BDP	A	2002	12/13	0.96	0.07	-	26,28,35,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GNS	B	1404[B]	15/16	0.92	0.13	-	30,36,37,39	15
5	NPO	B	1408[A]	7/10	0.72	0.23	-	44,53,58,63	7
8	EDO	A	2019[A]	4/4	0.90	0.29	-	26,28,31,33	4
8	EDO	A	2023	4/4	0.90	0.28	-	39,39,51,51	4
10	NA	B	1420	1/1	0.74	0.13	-	53,53,53,53	1
10	NA	A	2026	1/1	0.81	0.25	-	53,53,53,53	0
2	GNS	B	1406[A]	15/16	0.90	0.16	-	48,54,64,72	15
8	EDO	A	2019[B]	4/4	0.90	0.29	-	25,31,31,32	4
2	GNS	A	2005	15/16	0.93	0.21	-	43,54,76,87	0
10	NA	A	2028	1/1	0.94	0.09	-	48,48,48,48	0
2	GNS	A	2003	15/16	0.97	0.12	-	35,40,46,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.