



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2017 – 02:17 PM EDT

PDB ID : 5V0T
Title : Crystal structure of an alpha,alpha-trehalose-phosphate synthase (UDP-forming) from Burkholderia xenovorans in complex with glucose-6-phosphate
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2017-02-28
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-20029077
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-20029077

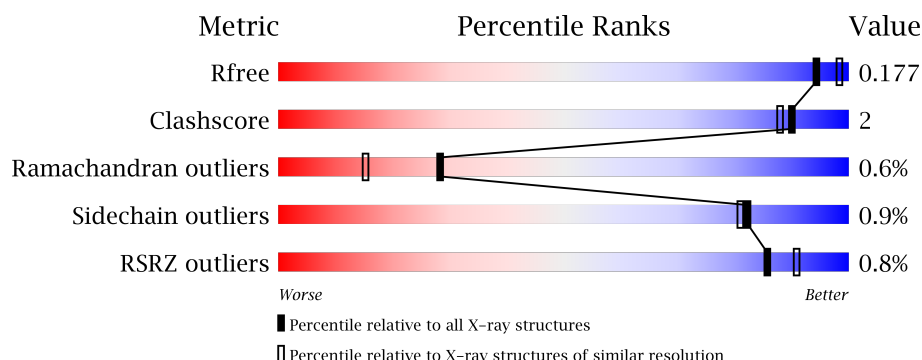
1 Overall quality at a glance

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	494	
1	B	494	
1	C	494	
1	D	494	
1	E	494	

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Mol	Chain	Length	Quality of chain
1	F	494	
1	G	494	
1	H	494	

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	EDO	A	504	-	-	-	X
4	EDO	B	504	-	-	-	X
4	EDO	C	503	-	-	-	X
4	EDO	C	504	-	-	-	X
4	EDO	D	503	-	-	-	X
4	EDO	D	504	-	-	-	X
4	EDO	F	503	-	-	-	X
4	EDO	H	503	-	-	-	X
4	EDO	H	504	-	-	-	X
5	ACT	A	505	-	-	-	X
5	ACT	B	505	-	-	-	X
5	ACT	B	506	-	-	-	X
5	ACT	B	508	-	-	-	X
5	ACT	C	505	-	-	-	X
5	ACT	D	505	-	-	-	X
5	ACT	D	506	-	-	X	-
5	ACT	F	504	-	-	-	X
5	ACT	G	504	-	-	-	X
5	ACT	H	505	-	-	-	X
6	OXD	A	507	-	-	-	X
6	OXD	B	510	-	-	-	X
6	OXD	E	506[A]	-	-	-	X
6	OXD	E	506[B]	-	-	-	X
6	OXD	F	506	-	-	-	X
7	FMT	A	509	-	-	-	X
7	FMT	A	513	-	-	-	X
7	FMT	B	512	-	-	-	X
7	FMT	B	514	-	-	-	X
7	FMT	C	507	-	-	-	X
7	FMT	D	507	-	-	-	X
7	FMT	D	509	-	-	-	X
7	FMT	F	507	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	TAR	E	503	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 32349 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 Alpha,alpha-trehalose-phosphate synthase (UDP-forming).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	9	0
			3619	2309	651	646	13			
1	B	453	Total	C	N	O	S	0	17	0
			3669	2341	659	656	13			
1	C	452	Total	C	N	O	S	0	3	0
			3588	2292	645	638	13			
1	D	452	Total	C	N	O	S	0	8	0
			3626	2317	657	639	13			
1	E	457	Total	C	N	O	S	0	12	0
			3664	2338	658	655	13			
1	F	455	Total	C	N	O	S	0	9	0
			3637	2321	658	645	13			
1	G	454	Total	C	N	O	S	0	12	0
			3567	2281	638	635	13			
1	H	451	Total	C	N	O	S	0	10	0
			3538	2261	632	632	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q13W28
A	2	ALA	-	expression tag	UNP Q13W28
A	3	HIS	-	expression tag	UNP Q13W28
A	4	HIS	-	expression tag	UNP Q13W28
A	5	HIS	-	expression tag	UNP Q13W28
A	6	HIS	-	expression tag	UNP Q13W28
A	7	HIS	-	expression tag	UNP Q13W28
A	8	HIS	-	expression tag	UNP Q13W28
B	1	MET	-	initiating methionine	UNP Q13W28
B	2	ALA	-	expression tag	UNP Q13W28
B	3	HIS	-	expression tag	UNP Q13W28
B	4	HIS	-	expression tag	UNP Q13W28
B	5	HIS	-	expression tag	UNP Q13W28

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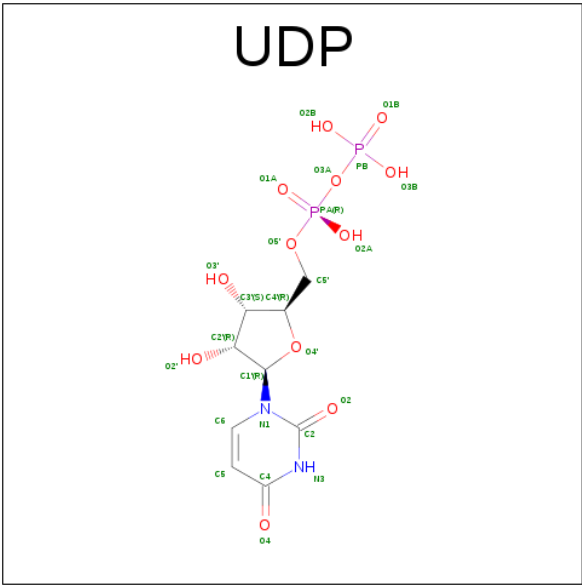
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP Q13W28
B	7	HIS	-	expression tag	UNP Q13W28
B	8	HIS	-	expression tag	UNP Q13W28
C	1	MET	-	initiating methionine	UNP Q13W28
C	2	ALA	-	expression tag	UNP Q13W28
C	3	HIS	-	expression tag	UNP Q13W28
C	4	HIS	-	expression tag	UNP Q13W28
C	5	HIS	-	expression tag	UNP Q13W28
C	6	HIS	-	expression tag	UNP Q13W28
C	7	HIS	-	expression tag	UNP Q13W28
C	8	HIS	-	expression tag	UNP Q13W28
D	1	MET	-	initiating methionine	UNP Q13W28
D	2	ALA	-	expression tag	UNP Q13W28
D	3	HIS	-	expression tag	UNP Q13W28
D	4	HIS	-	expression tag	UNP Q13W28
D	5	HIS	-	expression tag	UNP Q13W28
D	6	HIS	-	expression tag	UNP Q13W28
D	7	HIS	-	expression tag	UNP Q13W28
D	8	HIS	-	expression tag	UNP Q13W28
E	1	MET	-	initiating methionine	UNP Q13W28
E	2	ALA	-	expression tag	UNP Q13W28
E	3	HIS	-	expression tag	UNP Q13W28
E	4	HIS	-	expression tag	UNP Q13W28
E	5	HIS	-	expression tag	UNP Q13W28
E	6	HIS	-	expression tag	UNP Q13W28
E	7	HIS	-	expression tag	UNP Q13W28
E	8	HIS	-	expression tag	UNP Q13W28
F	1	MET	-	initiating methionine	UNP Q13W28
F	2	ALA	-	expression tag	UNP Q13W28
F	3	HIS	-	expression tag	UNP Q13W28
F	4	HIS	-	expression tag	UNP Q13W28
F	5	HIS	-	expression tag	UNP Q13W28
F	6	HIS	-	expression tag	UNP Q13W28
F	7	HIS	-	expression tag	UNP Q13W28
F	8	HIS	-	expression tag	UNP Q13W28
G	1	MET	-	initiating methionine	UNP Q13W28
G	2	ALA	-	expression tag	UNP Q13W28
G	3	HIS	-	expression tag	UNP Q13W28
G	4	HIS	-	expression tag	UNP Q13W28
G	5	HIS	-	expression tag	UNP Q13W28
G	6	HIS	-	expression tag	UNP Q13W28
G	7	HIS	-	expression tag	UNP Q13W28

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Chain	Residue	Modelled	Actual	Comment	Reference
G	8	HIS	-	expression tag	UNP Q13W28
H	1	MET	-	initiating methionine	UNP Q13W28
H	2	ALA	-	expression tag	UNP Q13W28
H	3	HIS	-	expression tag	UNP Q13W28
H	4	HIS	-	expression tag	UNP Q13W28
H	5	HIS	-	expression tag	UNP Q13W28
H	6	HIS	-	expression tag	UNP Q13W28
H	7	HIS	-	expression tag	UNP Q13W28
H	8	HIS	-	expression tag	UNP Q13W28

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: C₉H₁₄N₂O₁₂P₂).



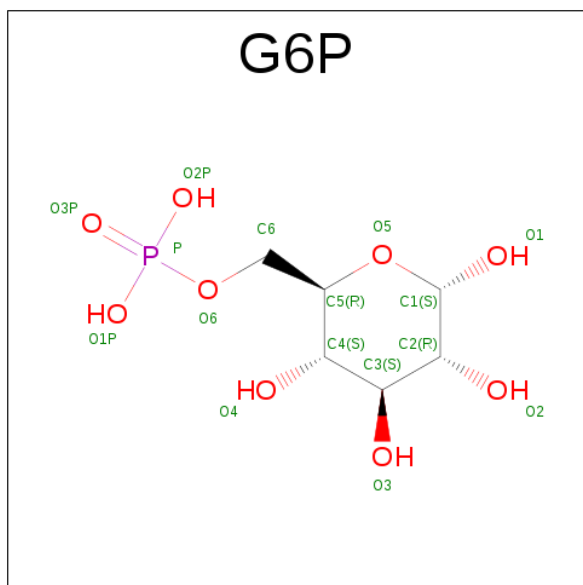
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	E	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	F	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	G	1	Total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

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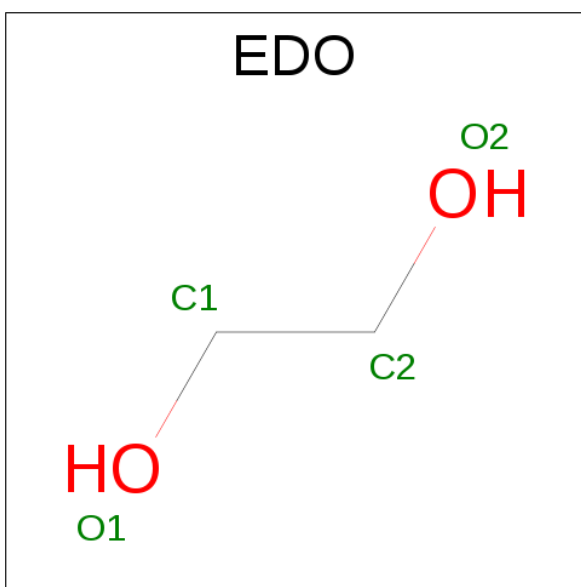
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is 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		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



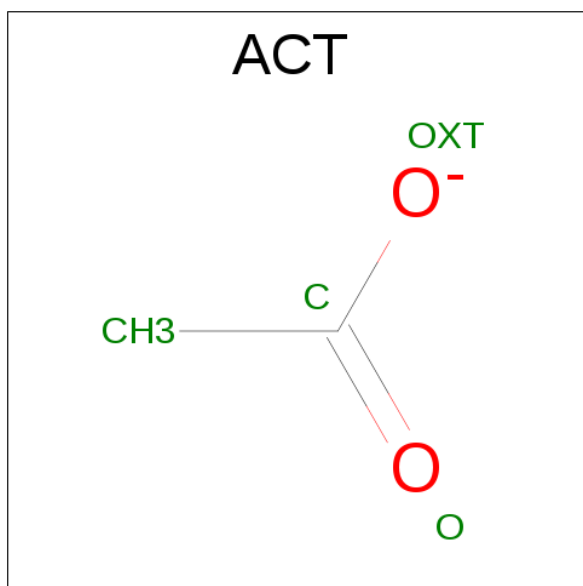
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



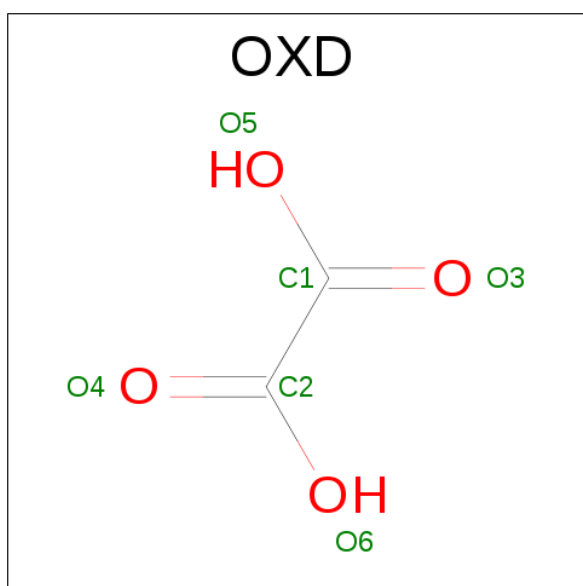
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total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

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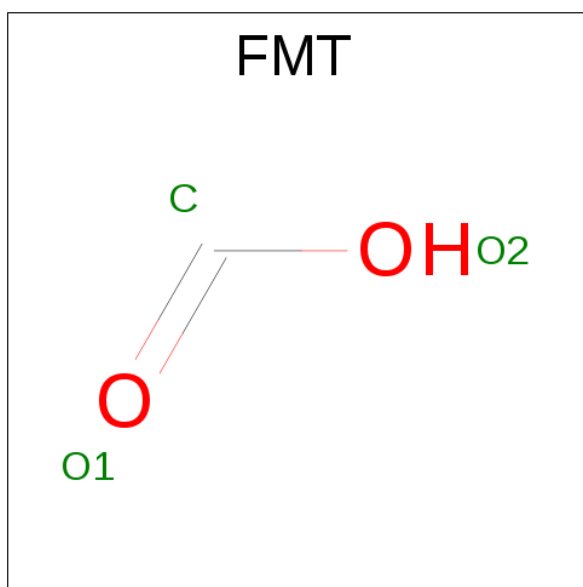
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is OXALIC ACID (three-letter code: OXD) (formula: $C_2H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	2	4		
6	B	1	Total	C	O	0	0
			6	2	4		
6	C	1	Total	C	O	0	0
			6	2	4		
6	E	1	Total	C	O	0	1
			12	4	8		
6	F	1	Total	C	O	0	0
			6	2	4		

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



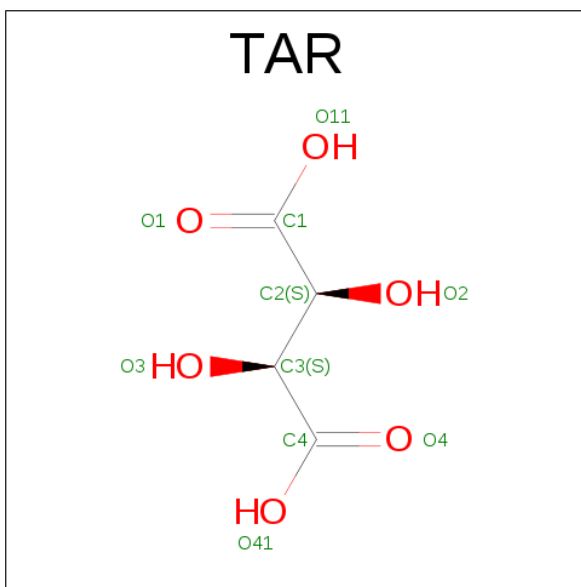
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	C	1	Total	C	O	0	0
			3	1	2		
7	C	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			3	1	2		
7	D	1	Total	C	O	0	0
			3	1	2		
7	D	1	Total	C	O	0	0
			3	1	2		
7	D	1	Total	C	O	0	0
			3	1	2		
7	E	1	Total	C	O	0	0
			3	1	2		
7	E	1	Total	C	O	0	0
			3	1	2		
7	E	1	Total	C	O	0	0
			3	1	2		
7	E	1	Total	C	O	0	0
			3	1	2		
7	F	1	Total	C	O	0	0
			3	1	2		
7	F	1	Total	C	O	0	0
			3	1	2		
7	F	1	Total	C	O	0	0
			3	1	2		
7	H	1	Total	C	O	0	0
			3	1	2		
7	H	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	C	O	0	0
			10	4	6		

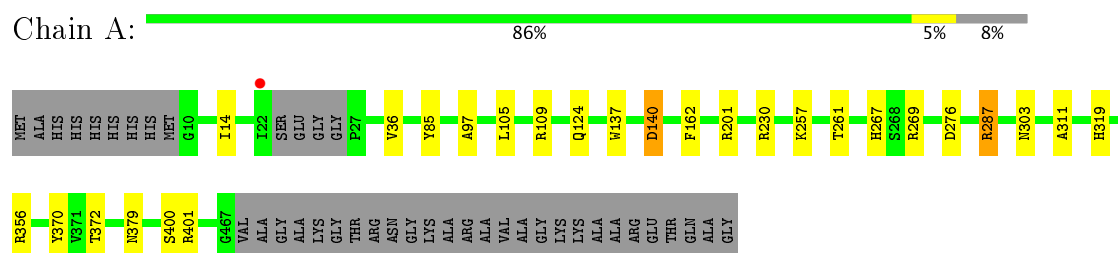
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	423	Total	O	0	2
			425	425		
9	B	401	Total	O	0	4
			404	404		
9	C	413	Total	O	0	2
			415	415		
9	D	395	Total	O	0	2
			397	397		
9	E	383	Total	O	0	2
			385	385		
9	F	368	Total	O	0	2
			370	370		
9	G	253	Total	O	0	2
			255	255		
9	H	214	Total	O	0	1
			215	215		

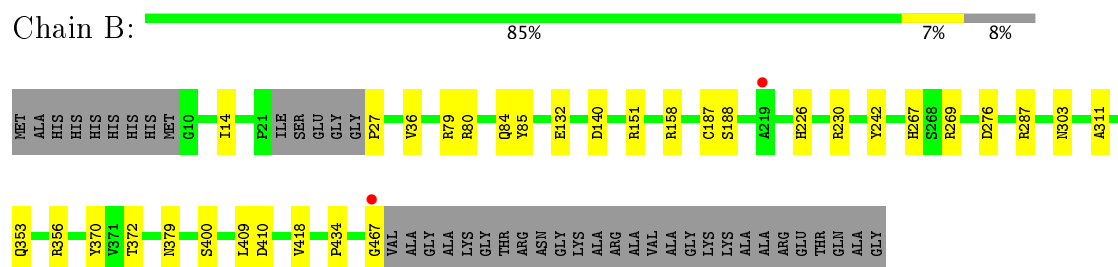
3 Residue-property plots [i](#)

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.

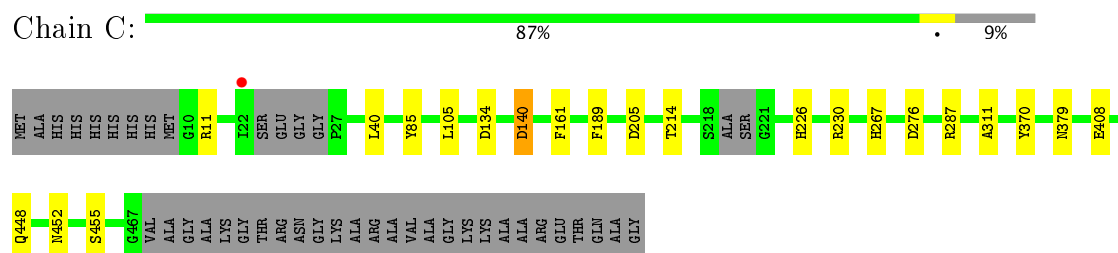
- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)



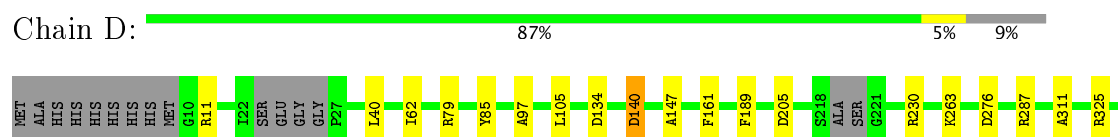
- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

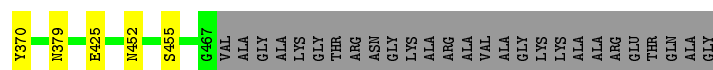


- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

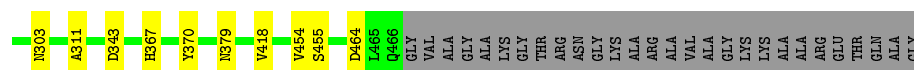
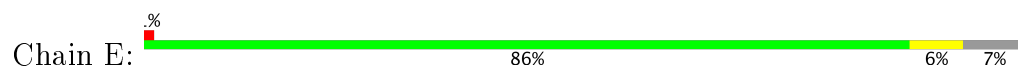


- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)

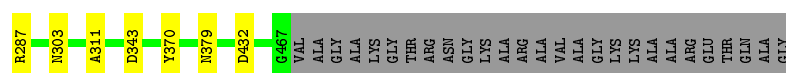
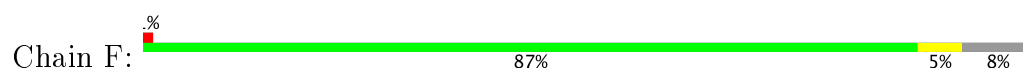




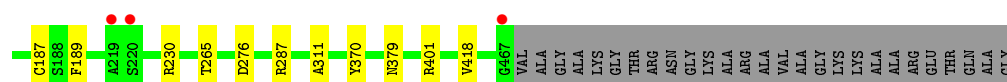
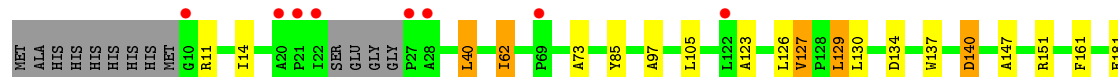
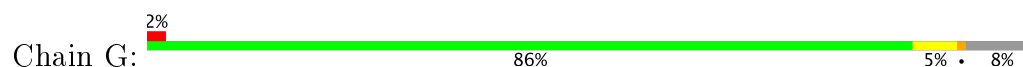
- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)



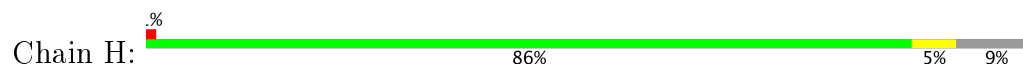
- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)



- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)



- Molecule 1: Alpha,alpha-trehalose-phosphate synthase (UDP-forming)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.92Å 105.95Å 135.71Å 91.36° 90.37° 89.97°	Depositor
Resolution (Å)	50.00 – 1.95 47.88 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-1.95) 93.3 (47.88-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.155 , 0.178 0.154 , 0.177	Depositor DCC
R_{free} test set	1979 reflections (0.60%)	DCC
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.408 for h,-k,-l 0.016 for -h,k,-l 0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32349	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: UDP, TAR, FMT, EDO, ACT, OXD, 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	0.39	0/3735	0.56	1/5076 (0.0%)
1	B	0.38	0/3797	0.58	2/5156 (0.0%)
1	C	0.38	0/3685	0.55	1/5005 (0.0%)
1	D	0.37	0/3739	0.54	1/5075 (0.0%)
1	E	0.38	0/3790	0.55	0/5149
1	F	0.37	0/3751	0.54	0/5094
1	G	0.34	0/3690	0.52	0/5022
1	H	0.33	0/3655	0.50	0/4977
All	All	0.37	0/29842	0.54	5/40554 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410[A]	ASP	C-N-CA	8.36	139.86	122.30
1	B	410[B]	ASP	C-N-CA	8.36	139.86	122.30
1	C	40	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	287	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	D	40	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	409	LEU	Peptide

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	3619	0	3568	15	0
1	B	3669	0	3627	20	0
1	C	3588	0	3542	10	0
1	D	3626	0	3598	14	0
1	E	3664	0	3629	18	0
1	F	3637	0	3593	17	0
1	G	3567	0	3482	21	0
1	H	3538	0	3422	14	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
2	C	25	0	11	0	0
2	D	25	0	11	0	0
2	E	25	0	11	0	0
2	F	25	0	11	0	0
2	G	25	0	11	0	0
2	H	25	0	11	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	0	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	0	0
4	A	8	0	12	0	0
4	B	12	0	18	0	0
4	C	8	0	12	0	0
4	D	8	0	12	1	0
4	E	8	0	12	0	0
4	F	4	0	6	0	0
4	G	4	0	6	0	0
4	H	8	0	12	0	0
5	A	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	20	0	15	0	0
5	C	4	0	3	0	0
5	D	8	0	6	2	0
5	E	4	0	3	0	0
5	F	8	0	6	0	0
5	G	4	0	3	0	0
5	H	4	0	3	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	C	6	0	0	0	0
6	E	12	0	0	0	0
6	F	6	0	0	1	0
7	A	18	0	6	1	0
7	B	18	0	6	2	0
7	C	6	0	2	0	0
7	D	12	0	4	0	0
7	E	12	0	4	1	0
7	F	9	0	3	0	0
7	H	6	0	2	0	0
8	E	10	0	4	1	0
9	A	425	0	0	4	0
9	B	404	0	0	4	0
9	C	415	0	0	1	0
9	D	397	0	0	6	0
9	E	385	0	0	3	0
9	F	370	0	0	4	0
9	G	255	0	0	1	0
9	H	215	0	0	0	0
All	All	32349	0	28803	124	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 (124) 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:27:PRO:O	1:B:353:GLN:NE2	2.10	0.84
1:B:356:ARG:NH2	9:B:601:HOH:O	2.05	0.82
1:B:230[A]:ARG:NH1	9:B:603:HOH:O	2.18	0.75
1:E:343:ASP:HA	1:H:265[B]:THR:HG21	1.69	0.74
1:A:356:ARG:NH2	9:A:601:HOH:O	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:ILE:HD11	1:G:73:ALA:HB1	1.72	0.71
1:E:212[A]:ASN:ND2	9:E:603:HOH:O	2.26	0.69
1:D:230:ARG:NH1	9:D:602:HOH:O	2.25	0.68
1:A:230:ARG:NH1	9:A:602:HOH:O	2.28	0.67
1:F:267:HIS:O	1:F:267:HIS:ND1	2.31	0.64
1:F:343:ASP:HA	1:G:265[B]:THR:HG21	1.78	0.64
1:B:353:GLN:OE1	9:B:602:HOH:O	2.16	0.62
1:D:425:GLU:OE1	9:D:601:HOH:O	2.16	0.61
1:D:325:ARG:HH22	5:D:506:ACT:H2	1.65	0.60
1:H:60:PRO:HB2	1:H:75:ILE:HG12	1.84	0.60
1:F:432:ASP:OD2	9:F:601:HOH:O	2.17	0.59
1:C:105:LEU:HD22	1:G:418:VAL:HG11	1.83	0.59
1:A:105:LEU:HD22	1:E:418:VAL:HG11	1.85	0.59
1:E:187:CYS:O	1:E:230:ARG:HD3	2.04	0.58
1:E:233:ARG:NH1	1:E:464:ASP:O	2.38	0.57
1:H:276:ASP:O	1:H:311:ALA:HA	2.05	0.57
1:E:242:TYR:HH	1:E:455[A]:SER:HG	1.53	0.56
1:G:127:VAL:HA	1:G:130:LEU:HD12	1.87	0.56
1:G:276:ASP:O	1:G:311:ALA:HA	2.06	0.55
1:G:401[B]:ARG:HG3	1:G:401[B]:ARG:HH21	1.72	0.55
1:D:263:LYS:NZ	9:D:849[B]:HOH:O	2.37	0.54
6:F:506:OXD:O4	9:F:602:HOH:O	2.18	0.54
1:A:401:ARG:NH2	9:A:607:HOH:O	2.42	0.52
1:C:230:ARG:NH1	9:C:601:HOH:O	2.18	0.51
1:H:11:ARG:HB3	1:H:134:ASP:OD1	2.11	0.51
1:D:287:ARG:HG3	1:D:370:TYR:CE2	2.45	0.51
1:H:97:ALA:HB2	1:H:105:LEU:HD12	1.91	0.51
1:C:276:ASP:O	1:C:311:ALA:HA	2.11	0.51
1:G:14:ILE:HD13	1:G:137:TRP:HB3	1.93	0.51
1:G:181:GLU:OE1	1:G:181:GLU:N	2.39	0.51
1:E:79:ARG:NH1	9:E:605:HOH:O	2.38	0.50
1:A:97:ALA:HB2	1:A:105:LEU:HD12	1.93	0.50
1:D:79:ARG:NH1	9:D:604:HOH:O	2.29	0.50
1:A:319:HIS:H	7:A:508:FMT:C	2.24	0.50
1:D:276:ASP:O	1:D:311:ALA:HA	2.12	0.50
4:D:504:EDO:H21	1:H:103:ASP:HA	1.93	0.49
1:E:11:ARG:HB3	1:E:134:ASP:OD1	2.12	0.49
1:G:187:CYS:O	1:G:230:ARG:HD3	2.12	0.49
1:F:276:ASP:O	1:F:311:ALA:HA	2.13	0.49
1:F:11:ARG:HB3	1:F:134:ASP:OD1	2.13	0.48
1:F:187:CYS:O	1:F:230:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ASP:O	1:E:311:ALA:HA	2.14	0.48
1:G:147:ALA:HB2	1:G:189:PHE:CE1	2.48	0.48
5:D:506:ACT:H1	9:D:946:HOH:O	2.13	0.48
1:G:147:ALA:O	1:G:151:ARG:HG2	2.13	0.48
1:B:434:PRO:HG2	1:D:425:GLU:HG2	1.96	0.47
1:B:226:HIS:HD2	9:B:638:HOH:O	1.97	0.47
1:G:161:PHE:HB2	1:G:189:PHE:CE1	2.49	0.47
1:C:214:THR:OG1	1:C:226:HIS:HB2	2.14	0.47
1:F:161:PHE:HB2	1:F:189:PHE:CE1	2.50	0.47
1:H:261:THR:O	1:H:265[B]:THR:HG23	2.15	0.47
1:B:269:ARG:NH2	1:B:303:ASN:OD1	2.48	0.47
1:B:276:ASP:O	1:B:311:ALA:HA	2.15	0.47
1:G:97:ALA:HB2	1:G:105:LEU:HD12	1.95	0.47
1:C:287:ARG:HG3	1:C:370:TYR:CZ	2.51	0.46
1:H:147:ALA:HB2	1:H:189:PHE:CE1	2.49	0.46
1:A:276:ASP:O	1:A:311:ALA:HA	2.15	0.46
1:B:158:ARG:NH2	1:B:467:GLY:O	2.49	0.46
8:E:503:TAR:O11	8:E:503:TAR:O3	2.29	0.46
1:G:11:ARG:HB3	1:G:134:ASP:OD1	2.15	0.45
1:F:176:VAL:HG12	1:F:178:PRO:HD2	1.97	0.45
1:A:201[B]:ARG:NH2	7:E:509:FMT:H	2.32	0.45
1:C:161:PHE:HB2	1:C:189:PHE:CE1	2.52	0.45
1:E:205[B]:ASP:OD1	9:E:601:HOH:O	2.21	0.45
1:E:271:LEU:H	1:E:367:HIS:HD1	1.64	0.45
1:B:418[A]:VAL:HG11	1:F:105:LEU:HD22	1.97	0.45
1:A:257:LYS:O	1:A:261:THR:HG23	2.18	0.44
1:D:11:ARG:HB3	1:D:134:ASP:OD1	2.17	0.44
1:H:161:PHE:HB2	1:H:189:PHE:CE1	2.52	0.44
1:H:319:HIS:NE2	1:H:323:ASP:OD2	2.50	0.44
1:B:79:ARG:NH1	7:B:513:FMT:O1	2.47	0.44
1:C:408:GLU:OE1	1:C:448:GLN:NE2	2.50	0.44
1:H:181:GLU:N	1:H:181:GLU:OE1	2.46	0.44
1:A:287:ARG:HG3	1:A:370:TYR:CZ	2.53	0.44
1:C:448:GLN:NE2	1:C:452:ASN:OD1	2.51	0.44
1:B:14:ILE:HG21	1:B:36:VAL:HG11	1.99	0.43
1:G:401[A]:ARG:NH2	9:G:606:HOH:O	2.51	0.43
1:A:124:GLN:HG2	9:A:638:HOH:O	2.18	0.43
1:D:97:ALA:HB2	1:D:105:LEU:HD12	1.99	0.43
1:A:14:ILE:HG21	1:A:36:VAL:HG11	2.00	0.43
1:C:287:ARG:HG3	1:C:370:TYR:CE2	2.53	0.43
1:E:217:PRO:HA	1:E:223:LEU:HD22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:ASP:CA	1:H:265[B]:THR:HG21	2.45	0.43
1:F:15:VAL:HG12	1:F:143:LEU:HD13	2.01	0.43
1:F:343:ASP:CA	1:G:265[B]:THR:HG21	2.48	0.43
1:H:147:ALA:HB2	1:H:189:PHE:CD1	2.54	0.43
1:F:79:ARG:NH1	9:F:608:HOH:O	2.41	0.43
1:A:269:ARG:NH1	1:A:303:ASN:OD1	2.52	0.42
1:E:287:ARG:HG3	1:E:370:TYR:CZ	2.53	0.42
1:B:287:ARG:HG3	1:B:370:TYR:CE2	2.53	0.42
1:F:269:ARG:NH2	1:F:303:ASN:OD1	2.49	0.42
1:G:40:LEU:HA	1:G:40:LEU:HD12	1.84	0.42
1:B:242:TYR:CZ	7:B:516:FMT:H	2.55	0.42
1:E:215:ALA:O	1:E:217:PRO:HD3	2.19	0.42
1:F:287:ARG:HG3	1:F:370:TYR:CZ	2.54	0.42
1:D:452:ASN:ND2	9:D:623:HOH:O	2.52	0.42
1:D:287:ARG:HG3	1:D:370:TYR:CZ	2.55	0.42
1:E:269:ARG:NH2	1:E:303:ASN:OD1	2.52	0.42
1:D:147:ALA:HB2	1:D:189:PHE:CE1	2.56	0.41
1:G:161:PHE:HB2	1:G:189:PHE:CD1	2.56	0.41
1:B:80:ARG:HE	1:B:84:GLN:HE22	1.67	0.41
1:A:372:THR:HA	1:A:400:SER:HB2	2.02	0.41
1:D:161:PHE:HB2	1:D:189:PHE:CE1	2.56	0.41
1:G:126:LEU:HA	1:G:129:LEU:HD12	2.01	0.41
1:B:372:THR:HA	1:B:400:SER:HB2	2.03	0.41
1:B:187:CYS:O	1:B:230[B]:ARG:NE	2.54	0.41
1:B:287:ARG:HG3	1:B:370:TYR:CZ	2.55	0.41
1:F:233:ARG:NH2	9:F:620:HOH:O	2.53	0.41
1:G:287:ARG:HG3	1:G:370:TYR:CZ	2.56	0.41
1:A:137:TRP:HE1	1:A:162:PHE:HB2	1.86	0.41
1:G:123:ALA:O	1:G:127:VAL:HG12	2.20	0.41
1:H:123:ALA:O	1:H:127:VAL:HG23	2.21	0.41
1:B:230[B]:ARG:HB3	1:B:230[B]:ARG:HE	1.46	0.41
1:C:11:ARG:HB3	1:C:134:ASP:OD1	2.21	0.41
1:F:287:ARG:HG3	1:F:370:TYR:CE2	2.56	0.41
1:E:161:PHE:HB2	1:E:189:PHE:CE1	2.56	0.41
1:E:38:ASP:HB3	1:E:454[A]:VAL:HG11	2.03	0.40
1:B:151[B]:ARG:NH1	1:B:188:SER:O	2.55	0.40
1:F:147:ALA:HB2	1:F:189:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/494 (93%)	443 (96%)	14 (3%)	3 (1%)	25	13
1	B	466/494 (94%)	450 (97%)	13 (3%)	3 (1%)	28	15
1	C	449/494 (91%)	434 (97%)	12 (3%)	3 (1%)	25	13
1	D	454/494 (92%)	438 (96%)	14 (3%)	2 (0%)	38	25
1	E	467/494 (94%)	447 (96%)	17 (4%)	3 (1%)	28	15
1	F	460/494 (93%)	444 (96%)	12 (3%)	4 (1%)	20	9
1	G	462/494 (94%)	447 (97%)	13 (3%)	2 (0%)	38	25
1	H	457/494 (92%)	445 (97%)	10 (2%)	2 (0%)	38	25
All	All	3675/3952 (93%)	3548 (96%)	105 (3%)	22 (1%)	28	15

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	21	PRO
1	A	379	ASN
1	B	267	HIS
1	B	379	ASN
1	C	267	HIS
1	C	379	ASN
1	D	379	ASN
1	E	379	ASN
1	F	379	ASN
1	G	379	ASN
1	H	379	ASN
1	A	140	ASP
1	A	267	HIS
1	B	140	ASP
1	F	140	ASP
1	C	140	ASP
1	E	140	ASP

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Mol	Chain	Res	Type
1	F	267	HIS
1	D	140	ASP
1	E	20	ALA
1	F	20	ALA
1	G	140	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/393 (94%)	367 (99%)	3 (1%)	85	83
1	B	377/393 (96%)	375 (100%)	2 (0%)	91	90
1	C	366/393 (93%)	362 (99%)	4 (1%)	78	75
1	D	371/393 (94%)	366 (99%)	5 (1%)	73	69
1	E	377/393 (96%)	375 (100%)	2 (0%)	91	90
1	F	371/393 (94%)	370 (100%)	1 (0%)	94	93
1	G	356/393 (91%)	350 (98%)	6 (2%)	66	60
1	H	350/393 (89%)	347 (99%)	3 (1%)	82	81
All	All	2938/3144 (93%)	2912 (99%)	26 (1%)	82	81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	TYR
1	A	109	ARG
1	A	140	ASP
1	B	85	TYR
1	B	132	GLU
1	C	85	TYR
1	C	140	ASP
1	C	205	ASP
1	C	455	SER
1	D	62	ILE

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Mol	Chain	Res	Type
1	D	85	TYR
1	D	140	ASP
1	D	205	ASP
1	D	455	SER
1	E	85	TYR
1	E	140	ASP
1	F	85	TYR
1	G	40	LEU
1	G	62	ILE
1	G	85	TYR
1	G	127	VAL
1	G	129	LEU
1	G	140	ASP
1	H	85	TYR
1	H	140	ASP
1	H	230	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	319	HIS
1	B	353	GLN
1	C	17	ASN
1	C	267	HIS
1	C	319	HIS
1	C	448	GLN
1	D	91	ASN
1	F	91	ASN
1	F	297	HIS
1	H	91	ASN
1	H	448	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

80 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	501	-	21,26,26	0.96	1 (4%)	22,40,40	3.30	2 (9%)
3	G6P	A	502	-	16,16,16	0.57	0	24,24,24	0.83	1 (4%)
4	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.41	0
4	EDO	A	504	-	3,3,3	0.58	0	2,2,2	0.14	0
5	ACT	A	505	-	1,3,3	6.19	1 (100%)	0,3,3	0.00	-
5	ACT	A	506	-	1,3,3	6.53	1 (100%)	0,3,3	0.00	-
6	OXD	A	507	-	0,5,5	0.00	-	0,6,6	0.00	-
7	FMT	A	508	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	509	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	510	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	511	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	512	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	513	-	0,2,2	0.00	-	0,1,1	0.00	-
2	UDP	B	501	-	21,26,26	0.91	1 (4%)	22,40,40	3.27	2 (9%)
3	G6P	B	502	-	16,16,16	0.57	0	24,24,24	0.67	0
4	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	B	504	-	3,3,3	0.51	0	2,2,2	0.21	0
5	ACT	B	505	-	1,3,3	6.65	1 (100%)	0,3,3	0.00	-
5	ACT	B	506	-	1,3,3	6.89	1 (100%)	0,3,3	0.00	-
5	ACT	B	507	-	1,3,3	6.92	1 (100%)	0,3,3	0.00	-
5	ACT	B	508	-	1,3,3	8.44	1 (100%)	0,3,3	0.00	-
5	ACT	B	509	-	1,3,3	7.20	1 (100%)	0,3,3	0.00	-
6	OXD	B	510	-	0,5,5	0.00	-	0,6,6	0.00	-
7	FMT	B	511	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	512	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FMT	B	513	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	514	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	515	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	516	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	B	517	-	3,3,3	0.50	0	2,2,2	0.26	0
2	UDP	C	501	-	21,26,26	0.96	1 (4%)	22,40,40	3.27	2 (9%)
3	G6P	C	502	-	16,16,16	0.65	0	24,24,24	1.02	1 (4%)
4	EDO	C	503	-	3,3,3	0.49	0	2,2,2	0.31	0
4	EDO	C	504	-	3,3,3	0.54	0	2,2,2	0.25	0
5	ACT	C	505	-	1,3,3	6.77	1 (100%)	0,3,3	0.00	-
6	OXD	C	506	-	0,5,5	0.00	-	0,6,6	0.00	-
7	FMT	C	507	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	C	508	-	0,2,2	0.00	-	0,1,1	0.00	-
2	UDP	D	501	-	21,26,26	0.89	1 (4%)	22,40,40	3.31	2 (9%)
3	G6P	D	502	-	16,16,16	0.58	0	24,24,24	1.11	2 (8%)
4	EDO	D	503	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	D	504	-	3,3,3	0.49	0	2,2,2	0.36	0
5	ACT	D	505	-	1,3,3	6.10	1 (100%)	0,3,3	0.00	-
5	ACT	D	506	-	1,3,3	5.01	1 (100%)	0,3,3	0.00	-
7	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	508	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	509	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	D	510	-	0,2,2	0.00	-	0,1,1	0.00	-
2	UDP	E	501	-	21,26,26	0.96	1 (4%)	22,40,40	3.27	2 (9%)
3	G6P	E	502	-	16,16,16	0.59	0	24,24,24	0.73	0
8	TAR	E	503	-	3,9,9	0.60	0	6,12,12	0.76	0
4	EDO	E	504	-	3,3,3	0.43	0	2,2,2	0.44	0
5	ACT	E	505	-	1,3,3	6.94	1 (100%)	0,3,3	0.00	-
6	OXD	E	506[A]	-	0,5,5	0.00	-	0,6,6	0.00	-
6	OXD	E	506[B]	-	0,5,5	0.00	-	0,6,6	0.00	-
7	FMT	E	507	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	508	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	509	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	E	510	-	0,2,2	0.00	-	0,1,1	0.00	-
4	EDO	E	511	-	3,3,3	0.50	0	2,2,2	0.47	0
2	UDP	F	501	-	21,26,26	0.93	1 (4%)	22,40,40	3.23	2 (9%)
3	G6P	F	502	-	16,16,16	0.50	0	24,24,24	0.66	0
4	EDO	F	503	-	3,3,3	0.45	0	2,2,2	0.28	0
5	ACT	F	504	-	1,3,3	7.31	1 (100%)	0,3,3	0.00	-
5	ACT	F	505	-	1,3,3	6.71	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	OXD	F	506	-	0,5,5	0.00	-	0,6,6	0.00	-
7	FMT	F	507	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	508	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	F	509	-	0,2,2	0.00	-	0,1,1	0.00	-
2	UDP	G	501	-	21,26,26	0.98	1 (4%)	22,40,40	3.31	2 (9%)
3	G6P	G	502	-	16,16,16	0.58	0	24,24,24	0.87	1 (4%)
4	EDO	G	503	-	3,3,3	0.49	0	2,2,2	0.28	0
5	ACT	G	504	-	1,3,3	7.34	1 (100%)	0,3,3	0.00	-
2	UDP	H	501	-	21,26,26	1.04	1 (4%)	22,40,40	3.29	2 (9%)
3	G6P	H	502	-	16,16,16	0.58	0	24,24,24	0.91	1 (4%)
4	EDO	H	503	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	H	504	-	3,3,3	0.56	0	2,2,2	0.17	0
5	ACT	H	505	-	1,3,3	7.02	1 (100%)	0,3,3	0.00	-
7	FMT	H	506	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	H	507	-	0,2,2	0.00	-	0,1,1	0.00	-

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	501	-	-	0/12/32/32	0/2/2/2
3	G6P	A	502	-	-	0/6/26/26	0/1/1/1
4	EDO	A	503	-	-	0/1/1/1	0/0/0/0
4	EDO	A	504	-	-	0/1/1/1	0/0/0/0
5	ACT	A	505	-	-	0/0/0/0	0/0/0/0
5	ACT	A	506	-	-	0/0/0/0	0/0/0/0
6	OXD	A	507	-	-	0/0/4/4	0/0/0/0
7	FMT	A	508	-	-	0/0/0/0	0/0/0/0
7	FMT	A	509	-	-	0/0/0/0	0/0/0/0
7	FMT	A	510	-	-	0/0/0/0	0/0/0/0
7	FMT	A	511	-	-	0/0/0/0	0/0/0/0
7	FMT	A	512	-	-	0/0/0/0	0/0/0/0
7	FMT	A	513	-	-	0/0/0/0	0/0/0/0
2	UDP	B	501	-	-	0/12/32/32	0/2/2/2
3	G6P	B	502	-	-	0/6/26/26	0/1/1/1
4	EDO	B	503	-	-	0/1/1/1	0/0/0/0
4	EDO	B	504	-	-	0/1/1/1	0/0/0/0
5	ACT	B	505	-	-	0/0/0/0	0/0/0/0
5	ACT	B	506	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ACT	B	507	-	-	0/0/0/0	0/0/0/0
5	ACT	B	508	-	-	0/0/0/0	0/0/0/0
5	ACT	B	509	-	-	0/0/0/0	0/0/0/0
6	OXD	B	510	-	-	0/0/4/4	0/0/0/0
7	FMT	B	511	-	-	0/0/0/0	0/0/0/0
7	FMT	B	512	-	-	0/0/0/0	0/0/0/0
7	FMT	B	513	-	-	0/0/0/0	0/0/0/0
7	FMT	B	514	-	-	0/0/0/0	0/0/0/0
7	FMT	B	515	-	-	0/0/0/0	0/0/0/0
7	FMT	B	516	-	-	0/0/0/0	0/0/0/0
4	EDO	B	517	-	-	0/1/1/1	0/0/0/0
2	UDP	C	501	-	-	0/12/32/32	0/2/2/2
3	G6P	C	502	-	-	0/6/26/26	0/1/1/1
4	EDO	C	503	-	-	0/1/1/1	0/0/0/0
4	EDO	C	504	-	-	0/1/1/1	0/0/0/0
5	ACT	C	505	-	-	0/0/0/0	0/0/0/0
6	OXD	C	506	-	-	0/0/4/4	0/0/0/0
7	FMT	C	507	-	-	0/0/0/0	0/0/0/0
7	FMT	C	508	-	-	0/0/0/0	0/0/0/0
2	UDP	D	501	-	-	0/12/32/32	0/2/2/2
3	G6P	D	502	-	-	0/6/26/26	0/1/1/1
4	EDO	D	503	-	-	0/1/1/1	0/0/0/0
4	EDO	D	504	-	-	0/1/1/1	0/0/0/0
5	ACT	D	505	-	-	0/0/0/0	0/0/0/0
5	ACT	D	506	-	-	0/0/0/0	0/0/0/0
7	FMT	D	507	-	-	0/0/0/0	0/0/0/0
7	FMT	D	508	-	-	0/0/0/0	0/0/0/0
7	FMT	D	509	-	-	0/0/0/0	0/0/0/0
7	FMT	D	510	-	-	0/0/0/0	0/0/0/0
2	UDP	E	501	-	-	0/12/32/32	0/2/2/2
3	G6P	E	502	-	-	0/6/26/26	0/1/1/1
8	TAR	E	503	-	-	0/4/12/12	0/0/0/0
4	EDO	E	504	-	-	0/1/1/1	0/0/0/0
5	ACT	E	505	-	-	0/0/0/0	0/0/0/0
6	OXD	E	506[A]	-	-	0/0/4/4	0/0/0/0
6	OXD	E	506[B]	-	-	0/0/4/4	0/0/0/0
7	FMT	E	507	-	-	0/0/0/0	0/0/0/0
7	FMT	E	508	-	-	0/0/0/0	0/0/0/0
7	FMT	E	509	-	-	0/0/0/0	0/0/0/0
7	FMT	E	510	-	-	0/0/0/0	0/0/0/0
4	EDO	E	511	-	-	0/1/1/1	0/0/0/0
2	UDP	F	501	-	-	0/12/32/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	F	502	-	-	0/6/26/26	0/1/1/1
4	EDO	F	503	-	-	0/1/1/1	0/0/0/0
5	ACT	F	504	-	-	0/0/0/0	0/0/0/0
5	ACT	F	505	-	-	0/0/0/0	0/0/0/0
6	OXD	F	506	-	-	0/0/4/4	0/0/0/0
7	FMT	F	507	-	-	0/0/0/0	0/0/0/0
7	FMT	F	508	-	-	0/0/0/0	0/0/0/0
7	FMT	F	509	-	-	0/0/0/0	0/0/0/0
2	UDP	G	501	-	-	0/12/32/32	0/2/2/2
3	G6P	G	502	-	-	0/6/26/26	0/1/1/1
4	EDO	G	503	-	-	0/1/1/1	0/0/0/0
5	ACT	G	504	-	-	0/0/0/0	0/0/0/0
2	UDP	H	501	-	-	0/12/32/32	0/2/2/2
3	G6P	H	502	-	-	0/6/26/26	0/1/1/1
4	EDO	H	503	-	-	0/1/1/1	0/0/0/0
4	EDO	H	504	-	-	0/1/1/1	0/0/0/0
5	ACT	H	505	-	-	0/0/0/0	0/0/0/0
7	FMT	H	506	-	-	0/0/0/0	0/0/0/0
7	FMT	H	507	-	-	0/0/0/0	0/0/0/0

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UDP	C4-N3	2.84	1.38	1.33
2	B	501	UDP	C4-N3	2.93	1.38	1.33
2	D	501	UDP	C4-N3	2.99	1.38	1.33
2	G	501	UDP	C4-N3	3.07	1.38	1.33
2	H	501	UDP	C4-N3	3.14	1.38	1.33
2	E	501	UDP	C4-N3	3.20	1.38	1.33
2	C	501	UDP	C4-N3	3.24	1.38	1.33
2	F	501	UDP	C4-N3	3.30	1.39	1.33
5	D	506	ACT	CH3-C	5.01	1.55	1.48
5	D	505	ACT	CH3-C	6.10	1.56	1.48
5	A	505	ACT	CH3-C	6.19	1.56	1.48
5	A	506	ACT	CH3-C	6.53	1.57	1.48
5	B	505	ACT	CH3-C	6.65	1.57	1.48
5	F	505	ACT	CH3-C	6.71	1.57	1.48
5	C	505	ACT	CH3-C	6.77	1.57	1.48
5	B	506	ACT	CH3-C	6.89	1.57	1.48
5	B	507	ACT	CH3-C	6.92	1.57	1.48
5	E	505	ACT	CH3-C	6.94	1.57	1.48
5	H	505	ACT	CH3-C	7.02	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	509	ACT	CH3-C	7.20	1.58	1.48
5	F	504	ACT	CH3-C	7.31	1.58	1.48
5	G	504	ACT	CH3-C	7.34	1.58	1.48
5	B	508	ACT	CH3-C	8.44	1.59	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	UDP	C5-C4-N3	-3.52	114.71	123.12
2	G	501	UDP	C5-C4-N3	-3.50	114.75	123.12
2	C	501	UDP	C5-C4-N3	-3.47	114.84	123.12
2	A	501	UDP	C5-C4-N3	-3.46	114.86	123.12
2	F	501	UDP	C5-C4-N3	-3.45	114.88	123.12
2	H	501	UDP	C5-C4-N3	-3.45	114.89	123.12
2	D	501	UDP	C5-C4-N3	-3.43	114.94	123.12
2	B	501	UDP	C5-C4-N3	-3.42	114.95	123.12
3	D	502	G6P	O1P-P-O6	-2.36	100.46	106.73
3	G	502	G6P	O5-C5-C6	2.53	111.69	106.64
3	A	502	G6P	O5-C5-C6	2.55	111.73	106.64
3	H	502	G6P	O5-C5-C6	2.56	111.76	106.64
3	D	502	G6P	O5-C5-C6	2.71	112.04	106.64
3	C	502	G6P	O5-C5-C6	2.94	112.51	106.64
2	C	501	UDP	C4-N3-C2	14.60	126.67	114.13
2	F	501	UDP	C4-N3-C2	14.62	126.69	114.13
2	E	501	UDP	C4-N3-C2	14.66	126.72	114.13
2	B	501	UDP	C4-N3-C2	14.69	126.75	114.13
2	H	501	UDP	C4-N3-C2	14.73	126.78	114.13
2	A	501	UDP	C4-N3-C2	14.82	126.86	114.13
2	D	501	UDP	C4-N3-C2	14.87	126.90	114.13
2	G	501	UDP	C4-N3-C2	14.91	126.94	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	508	FMT	1	0
7	B	513	FMT	1	0
7	B	516	FMT	1	0
4	D	504	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	506	ACT	2	0
8	E	503	TAR	1	0
7	E	509	FMT	1	0
6	F	506	OXD	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, 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	454/494 (91%)	-0.56	1 (0%) 94 97	15, 24, 46, 76	0
1	B	453/494 (91%)	-0.57	2 (0%) 92 95	16, 25, 46, 82	0
1	C	452/494 (91%)	-0.53	1 (0%) 94 97	16, 26, 47, 91	0
1	D	452/494 (91%)	-0.53	0 100 100	16, 27, 48, 95	0
1	E	457/494 (92%)	-0.43	6 (1%) 77 84	16, 27, 56, 95	0
1	F	455/494 (92%)	-0.42	4 (0%) 84 89	17, 28, 56, 76	0
1	G	454/494 (91%)	-0.23	11 (2%) 59 69	19, 39, 72, 106	0
1	H	451/494 (91%)	-0.17	5 (1%) 80 86	18, 41, 76, 97	0
All	All	3628/3952 (91%)	-0.43	30 (0%) 86 91	15, 29, 61, 106	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	219	ALA	5.5
1	E	10	GLY	4.9
1	G	467	GLY	4.4
1	B	219	ALA	4.0
1	E	27	PRO	3.6
1	H	22	ILE	3.5
1	H	219	ALA	3.3
1	G	21	PRO	3.0
1	F	27	PRO	2.9
1	E	28	ALA	2.8
1	G	22	ILE	2.8
1	H	220	SER	2.8
1	E	219	ALA	2.8
1	F	10	GLY	2.7
1	G	27	PRO	2.7
1	G	220	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	28	ALA	2.4
1	C	22	ILE	2.4
1	G	28	ALA	2.3
1	H	69	PRO	2.3
1	E	26	GLY	2.3
1	G	10	GLY	2.3
1	F	21	PRO	2.3
1	E	220	SER	2.3
1	G	20	ALA	2.2
1	A	22	ILE	2.2
1	B	467	GLY	2.2
1	G	69	PRO	2.1
1	G	122	LEU	2.1
1	H	467	GLY	2.1

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(Å ²)	Q<0.9
8	TAR	E	503	10/10	0.65	0.33	36.55	71,75,81,84	0
6	OXD	E	506[B]	6/6	0.94	0.22	30.29	56,57,58,59	6
6	OXD	E	506[A]	6/6	0.94	0.22	30.29	57,57,58,58	6
4	EDO	D	504	4/4	0.87	0.22	29.77	51,55,55,59	0
7	FMT	B	512	3/3	0.85	0.39	28.75	53,53,57,59	0
4	EDO	H	504	4/4	0.79	0.28	17.83	48,49,50,51	0
4	EDO	A	504	4/4	0.91	0.18	16.76	48,49,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	FMT	D	509	3/3	0.75	0.16	15.23	46,46,51,54	0
5	ACT	B	506	4/4	0.76	0.18	13.42	48,48,58,59	0
7	FMT	D	507	3/3	0.87	0.18	12.29	61,61,62,64	0
4	EDO	B	504	4/4	0.93	0.16	10.66	49,50,50,52	0
6	OXD	A	507	6/6	0.91	0.14	10.27	63,64,70,74	0
4	EDO	H	503	4/4	0.92	0.20	10.09	34,42,49,51	0
7	FMT	B	514	3/3	0.81	0.41	9.53	64,64,65,69	0
6	OXD	B	510	6/6	0.82	0.23	9.04	71,71,74,78	0
4	EDO	F	503	4/4	0.96	0.14	8.79	36,38,41,41	0
4	EDO	C	503	4/4	0.97	0.13	8.59	29,37,38,43	0
4	EDO	C	504	4/4	0.94	0.20	7.94	42,44,45,45	0
5	ACT	F	504	4/4	0.89	0.13	7.09	40,44,50,53	0
7	FMT	F	507	3/3	0.92	0.19	6.67	54,54,58,59	0
5	ACT	A	505	4/4	0.91	0.13	6.60	39,51,53,53	0
5	ACT	B	505	4/4	0.91	0.13	6.46	37,45,51,52	0
6	OXD	F	506	6/6	0.94	0.15	5.85	67,68,70,71	0
5	ACT	D	505	4/4	0.89	0.11	5.49	35,40,43,45	0
5	ACT	B	508	4/4	0.72	0.20	5.08	51,57,61,64	0
7	FMT	A	509	3/3	0.91	0.20	4.07	52,52,54,58	0
5	ACT	H	505	4/4	0.88	0.12	3.78	38,49,51,53	0
7	FMT	A	513	3/3	0.79	0.22	3.50	45,45,54,56	0
5	ACT	G	504	4/4	0.91	0.11	3.47	36,47,49,49	0
5	ACT	C	505	4/4	0.96	0.09	3.14	35,39,45,45	0
7	FMT	C	507	3/3	0.96	0.12	2.52	43,43,47,48	0
4	EDO	D	503	4/4	0.97	0.11	2.43	27,30,33,36	0
7	FMT	D	510	3/3	0.83	0.12	1.80	55,55,55,60	0
4	EDO	E	504	4/4	0.95	0.11	1.52	33,34,37,38	0
4	EDO	G	503	4/4	0.94	0.14	1.15	34,37,47,51	0
3	G6P	C	502	16/16	0.99	0.08	1.11	15,19,21,21	0
3	G6P	A	502	16/16	0.99	0.08	1.10	13,18,19,21	0
7	FMT	E	507	3/3	0.91	0.24	1.05	67,67,68,69	0
7	FMT	B	511	3/3	0.96	0.09	0.69	40,40,43,43	0
7	FMT	D	508	3/3	0.95	0.10	0.60	47,47,49,50	0
7	FMT	B	516	3/3	0.75	0.12	0.56	73,73,73,75	0
3	G6P	D	502	16/16	0.99	0.08	0.39	14,19,22,25	0
4	EDO	A	503	4/4	0.98	0.07	0.24	30,35,38,38	0
3	G6P	B	502	16/16	0.99	0.07	0.01	13,19,21,23	0
2	UDP	C	501	25/25	0.99	0.08	-0.14	14,18,21,21	0
2	UDP	B	501	25/25	0.99	0.08	-0.17	15,18,22,25	0
2	UDP	A	501	25/25	0.99	0.07	-0.36	14,18,23,23	0
3	G6P	G	502	16/16	0.97	0.07	-0.49	28,32,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	UDP	D	501	25/25	0.99	0.08	-0.51	15,18,21,22	0
2	UDP	H	501	25/25	0.99	0.09	-0.60	23,29,33,37	0
3	G6P	E	502	16/16	0.99	0.07	-0.61	19,23,25,26	0
2	UDP	G	501	25/25	0.98	0.08	-0.62	22,27,32,34	0
3	G6P	F	502	16/16	0.99	0.07	-0.70	19,24,30,30	0
2	UDP	E	501	25/25	0.99	0.07	-0.77	15,19,21,23	0
4	EDO	B	503	4/4	0.98	0.07	-0.84	27,32,35,41	0
2	UDP	F	501	25/25	0.99	0.07	-0.95	16,21,23,24	0
3	G6P	H	502	16/16	0.98	0.07	-1.10	31,34,41,43	0
7	FMT	F	508	3/3	0.95	0.08	-1.55	47,47,49,52	0
7	FMT	B	515	3/3	0.90	0.17	-	70,70,70,71	0
5	ACT	B	509	4/4	0.72	0.18	-	66,68,70,70	0
7	FMT	H	507	3/3	0.94	0.13	-	66,66,66,68	0
5	ACT	B	507	4/4	0.76	0.29	-	62,71,72,74	0
7	FMT	C	508	3/3	0.90	0.31	-	38,38,44,47	0
7	FMT	A	510	3/3	0.91	0.13	-	63,63,65,67	0
7	FMT	H	506	3/3	0.83	0.25	-	49,49,49,51	0
7	FMT	E	508	3/3	0.84	0.17	-	69,69,70,71	0
4	EDO	B	517	4/4	0.92	0.16	-	40,55,62,63	0
7	FMT	A	511	3/3	0.93	0.28	-	73,73,73,75	0
5	ACT	D	506	4/4	0.83	0.14	-	28,54,60,62	0
5	ACT	F	505	4/4	0.93	0.24	-	58,59,61,61	0
7	FMT	A	512	3/3	0.83	0.16	-	58,58,65,65	0
7	FMT	E	509	3/3	0.82	0.19	-	63,63,65,67	0
5	ACT	A	506	4/4	0.85	0.15	-	57,65,67,69	0
7	FMT	B	513	3/3	0.88	0.17	-	48,48,55,56	0
6	OXD	C	506	6/6	0.88	0.25	-	70,75,76,77	0
7	FMT	F	509	3/3	0.73	0.21	-	79,79,79,81	0
5	ACT	E	505	4/4	0.72	0.22	-	68,68,68,71	0
4	EDO	E	511	4/4	0.90	0.14	-	59,59,61,62	0
7	FMT	E	510	3/3	0.82	0.12	-	64,64,66,68	0
7	FMT	A	508	3/3	0.91	0.09	-	45,45,45,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.