Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 04:36 PM JST

PDB ID	:	4TVU
Title	:	Crystal structure of trehalose synthase from Deinococcus radiodurans reveals a closed conformation for catalysis of the intramolecular isomerization
Authors	:	Wang, Y.L.; Chow, S.Y.; Lin, Y.T.; Liaw, S.H.
Deposited on	:	2014-06-28
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

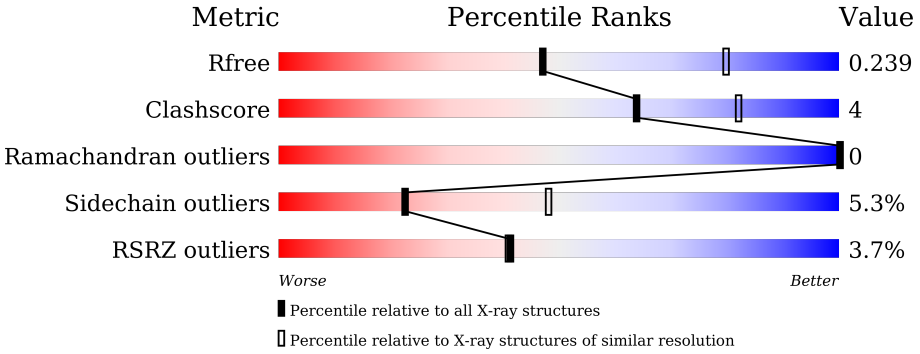
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	571	% 84% 9% • •
1	B	571	2% 85% 8% • •
1	C	571	4% 85% 8% • •
1	D	571	4% 86% 8% • •
1	E	571	% 86% 8% • •
1	F	571	4% 85% 8% • •

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Mol	Chain	Length	Quality of chain
1	G	571	2% 85% 9%
1	H	571	10% 83% 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 36291 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 Trehalose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	548	4404	2818	751	819	16	0	0	0
1	B	548	4404	2818	751	819	16	0	0	0
1	C	548	4404	2818	751	819	16	0	0	0
1	D	548	4404	2818	751	819	16	0	0	0
1	E	548	4404	2818	751	819	16	0	0	0
1	F	548	4404	2818	751	819	16	0	0	0
1	G	548	4404	2818	751	819	16	0	0	0
1	H	548	4404	2818	751	819	16	0	0	0

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP I3NX86
A	0	VAL	-	expression tag	UNP I3NX86
A	1	PRO	-	expression tag	UNP I3NX86
A	97	TRP	ARG	engineered mutation	UNP I3NX86
A	313	ILE	THR	engineered mutation	UNP I3NX86
A	380	VAL	ILE	engineered mutation	UNP I3NX86
A	553	SER	-	expression tag	UNP I3NX86
A	554	ARG	-	expression tag	UNP I3NX86
A	555	VAL	-	expression tag	UNP I3NX86
A	556	ASP	-	expression tag	UNP I3NX86
A	557	LYS	-	expression tag	UNP I3NX86
A	558	LEU	-	expression tag	UNP I3NX86
A	559	ALA	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
A	560	ALA	-	expression tag	UNP I3NX86
A	561	ALA	-	expression tag	UNP I3NX86
A	562	LEU	-	expression tag	UNP I3NX86
A	563	GLU	-	expression tag	UNP I3NX86
A	564	HIS	-	expression tag	UNP I3NX86
A	565	HIS	-	expression tag	UNP I3NX86
A	566	HIS	-	expression tag	UNP I3NX86
A	567	HIS	-	expression tag	UNP I3NX86
A	568	HIS	-	expression tag	UNP I3NX86
A	569	HIS	-	expression tag	UNP I3NX86
B	-1	MET	-	expression tag	UNP I3NX86
B	0	VAL	-	expression tag	UNP I3NX86
B	1	PRO	-	expression tag	UNP I3NX86
B	97	TRP	ARG	engineered mutation	UNP I3NX86
B	313	ILE	THR	engineered mutation	UNP I3NX86
B	380	VAL	ILE	engineered mutation	UNP I3NX86
B	553	SER	-	expression tag	UNP I3NX86
B	554	ARG	-	expression tag	UNP I3NX86
B	555	VAL	-	expression tag	UNP I3NX86
B	556	ASP	-	expression tag	UNP I3NX86
B	557	LYS	-	expression tag	UNP I3NX86
B	558	LEU	-	expression tag	UNP I3NX86
B	559	ALA	-	expression tag	UNP I3NX86
B	560	ALA	-	expression tag	UNP I3NX86
B	561	ALA	-	expression tag	UNP I3NX86
B	562	LEU	-	expression tag	UNP I3NX86
B	563	GLU	-	expression tag	UNP I3NX86
B	564	HIS	-	expression tag	UNP I3NX86
B	565	HIS	-	expression tag	UNP I3NX86
B	566	HIS	-	expression tag	UNP I3NX86
B	567	HIS	-	expression tag	UNP I3NX86
B	568	HIS	-	expression tag	UNP I3NX86
B	569	HIS	-	expression tag	UNP I3NX86
C	-1	MET	-	expression tag	UNP I3NX86
C	0	VAL	-	expression tag	UNP I3NX86
C	1	PRO	-	expression tag	UNP I3NX86
C	97	TRP	ARG	engineered mutation	UNP I3NX86
C	313	ILE	THR	engineered mutation	UNP I3NX86
C	380	VAL	ILE	engineered mutation	UNP I3NX86
C	553	SER	-	expression tag	UNP I3NX86
C	554	ARG	-	expression tag	UNP I3NX86
C	555	VAL	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
C	556	ASP	-	expression tag	UNP I3NX86
C	557	LYS	-	expression tag	UNP I3NX86
C	558	LEU	-	expression tag	UNP I3NX86
C	559	ALA	-	expression tag	UNP I3NX86
C	560	ALA	-	expression tag	UNP I3NX86
C	561	ALA	-	expression tag	UNP I3NX86
C	562	LEU	-	expression tag	UNP I3NX86
C	563	GLU	-	expression tag	UNP I3NX86
C	564	HIS	-	expression tag	UNP I3NX86
C	565	HIS	-	expression tag	UNP I3NX86
C	566	HIS	-	expression tag	UNP I3NX86
C	567	HIS	-	expression tag	UNP I3NX86
C	568	HIS	-	expression tag	UNP I3NX86
C	569	HIS	-	expression tag	UNP I3NX86
D	-1	MET	-	expression tag	UNP I3NX86
D	0	VAL	-	expression tag	UNP I3NX86
D	1	PRO	-	expression tag	UNP I3NX86
D	97	TRP	ARG	engineered mutation	UNP I3NX86
D	313	ILE	THR	engineered mutation	UNP I3NX86
D	380	VAL	ILE	engineered mutation	UNP I3NX86
D	553	SER	-	expression tag	UNP I3NX86
D	554	ARG	-	expression tag	UNP I3NX86
D	555	VAL	-	expression tag	UNP I3NX86
D	556	ASP	-	expression tag	UNP I3NX86
D	557	LYS	-	expression tag	UNP I3NX86
D	558	LEU	-	expression tag	UNP I3NX86
D	559	ALA	-	expression tag	UNP I3NX86
D	560	ALA	-	expression tag	UNP I3NX86
D	561	ALA	-	expression tag	UNP I3NX86
D	562	LEU	-	expression tag	UNP I3NX86
D	563	GLU	-	expression tag	UNP I3NX86
D	564	HIS	-	expression tag	UNP I3NX86
D	565	HIS	-	expression tag	UNP I3NX86
D	566	HIS	-	expression tag	UNP I3NX86
D	567	HIS	-	expression tag	UNP I3NX86
D	568	HIS	-	expression tag	UNP I3NX86
D	569	HIS	-	expression tag	UNP I3NX86
E	-1	MET	-	expression tag	UNP I3NX86
E	0	VAL	-	expression tag	UNP I3NX86
E	1	PRO	-	expression tag	UNP I3NX86
E	97	TRP	ARG	engineered mutation	UNP I3NX86
E	313	ILE	THR	engineered mutation	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
E	380	VAL	ILE	engineered mutation	UNP I3NX86
E	553	SER	-	expression tag	UNP I3NX86
E	554	ARG	-	expression tag	UNP I3NX86
E	555	VAL	-	expression tag	UNP I3NX86
E	556	ASP	-	expression tag	UNP I3NX86
E	557	LYS	-	expression tag	UNP I3NX86
E	558	LEU	-	expression tag	UNP I3NX86
E	559	ALA	-	expression tag	UNP I3NX86
E	560	ALA	-	expression tag	UNP I3NX86
E	561	ALA	-	expression tag	UNP I3NX86
E	562	LEU	-	expression tag	UNP I3NX86
E	563	GLU	-	expression tag	UNP I3NX86
E	564	HIS	-	expression tag	UNP I3NX86
E	565	HIS	-	expression tag	UNP I3NX86
E	566	HIS	-	expression tag	UNP I3NX86
E	567	HIS	-	expression tag	UNP I3NX86
E	568	HIS	-	expression tag	UNP I3NX86
E	569	HIS	-	expression tag	UNP I3NX86
F	-1	MET	-	expression tag	UNP I3NX86
F	0	VAL	-	expression tag	UNP I3NX86
F	1	PRO	-	expression tag	UNP I3NX86
F	97	TRP	ARG	engineered mutation	UNP I3NX86
F	313	ILE	THR	engineered mutation	UNP I3NX86
F	380	VAL	ILE	engineered mutation	UNP I3NX86
F	553	SER	-	expression tag	UNP I3NX86
F	554	ARG	-	expression tag	UNP I3NX86
F	555	VAL	-	expression tag	UNP I3NX86
F	556	ASP	-	expression tag	UNP I3NX86
F	557	LYS	-	expression tag	UNP I3NX86
F	558	LEU	-	expression tag	UNP I3NX86
F	559	ALA	-	expression tag	UNP I3NX86
F	560	ALA	-	expression tag	UNP I3NX86
F	561	ALA	-	expression tag	UNP I3NX86
F	562	LEU	-	expression tag	UNP I3NX86
F	563	GLU	-	expression tag	UNP I3NX86
F	564	HIS	-	expression tag	UNP I3NX86
F	565	HIS	-	expression tag	UNP I3NX86
F	566	HIS	-	expression tag	UNP I3NX86
F	567	HIS	-	expression tag	UNP I3NX86
F	568	HIS	-	expression tag	UNP I3NX86
F	569	HIS	-	expression tag	UNP I3NX86
G	-1	MET	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	VAL	-	expression tag	UNP I3NX86
G	1	PRO	-	expression tag	UNP I3NX86
G	97	TRP	ARG	engineered mutation	UNP I3NX86
G	313	ILE	THR	engineered mutation	UNP I3NX86
G	380	VAL	ILE	engineered mutation	UNP I3NX86
G	553	SER	-	expression tag	UNP I3NX86
G	554	ARG	-	expression tag	UNP I3NX86
G	555	VAL	-	expression tag	UNP I3NX86
G	556	ASP	-	expression tag	UNP I3NX86
G	557	LYS	-	expression tag	UNP I3NX86
G	558	LEU	-	expression tag	UNP I3NX86
G	559	ALA	-	expression tag	UNP I3NX86
G	560	ALA	-	expression tag	UNP I3NX86
G	561	ALA	-	expression tag	UNP I3NX86
G	562	LEU	-	expression tag	UNP I3NX86
G	563	GLU	-	expression tag	UNP I3NX86
G	564	HIS	-	expression tag	UNP I3NX86
G	565	HIS	-	expression tag	UNP I3NX86
G	566	HIS	-	expression tag	UNP I3NX86
G	567	HIS	-	expression tag	UNP I3NX86
G	568	HIS	-	expression tag	UNP I3NX86
G	569	HIS	-	expression tag	UNP I3NX86
H	-1	MET	-	expression tag	UNP I3NX86
H	0	VAL	-	expression tag	UNP I3NX86
H	1	PRO	-	expression tag	UNP I3NX86
H	97	TRP	ARG	engineered mutation	UNP I3NX86
H	313	ILE	THR	engineered mutation	UNP I3NX86
H	380	VAL	ILE	engineered mutation	UNP I3NX86
H	553	SER	-	expression tag	UNP I3NX86
H	554	ARG	-	expression tag	UNP I3NX86
H	555	VAL	-	expression tag	UNP I3NX86
H	556	ASP	-	expression tag	UNP I3NX86
H	557	LYS	-	expression tag	UNP I3NX86
H	558	LEU	-	expression tag	UNP I3NX86
H	559	ALA	-	expression tag	UNP I3NX86
H	560	ALA	-	expression tag	UNP I3NX86
H	561	ALA	-	expression tag	UNP I3NX86
H	562	LEU	-	expression tag	UNP I3NX86
H	563	GLU	-	expression tag	UNP I3NX86
H	564	HIS	-	expression tag	UNP I3NX86
H	565	HIS	-	expression tag	UNP I3NX86
H	566	HIS	-	expression tag	UNP I3NX86

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Chain	Residue	Modelled	Actual	Comment	Reference
H	567	HIS	-	expression tag	UNP I3NX86
H	568	HIS	-	expression tag	UNP I3NX86
H	569	HIS	-	expression tag	UNP I3NX86

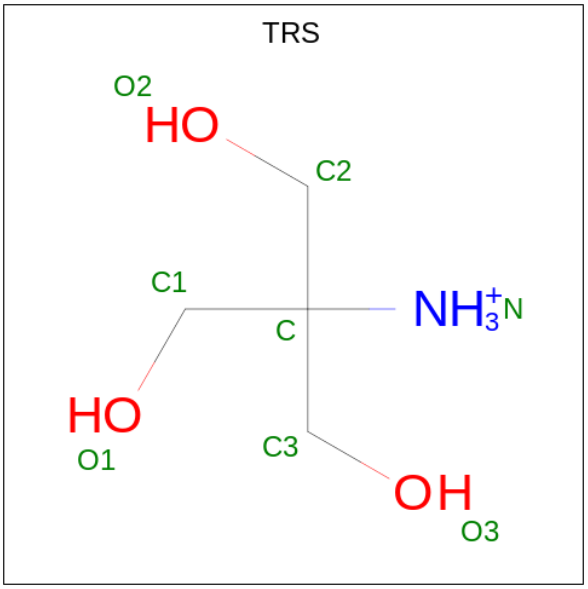
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0
4	B	1	8	4	1	3	0	0
4	C	1	8	4	1	3	0	0
4	D	1	8	4	1	3	0	0
4	E	1	8	4	1	3	0	0
4	F	1	8	4	1	3	0	0
4	G	1	8	4	1	3	0	0
4	H	1	8	4	1	3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	157	157	157	0	0
5	B	147	147	147	0	0

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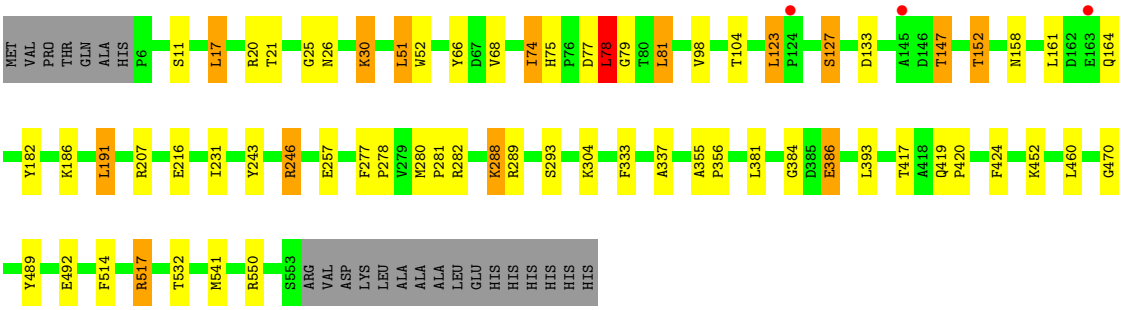
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	C	107	107	107	0	0
			Total	O		
5	D	99	99	99	0	0
			Total	O		
5	E	193	193	193	0	0
			Total	O		
5	F	85	85	85	0	0
			Total	O		
5	G	133	133	133	0	0
			Total	O		
5	H	58	58	58	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

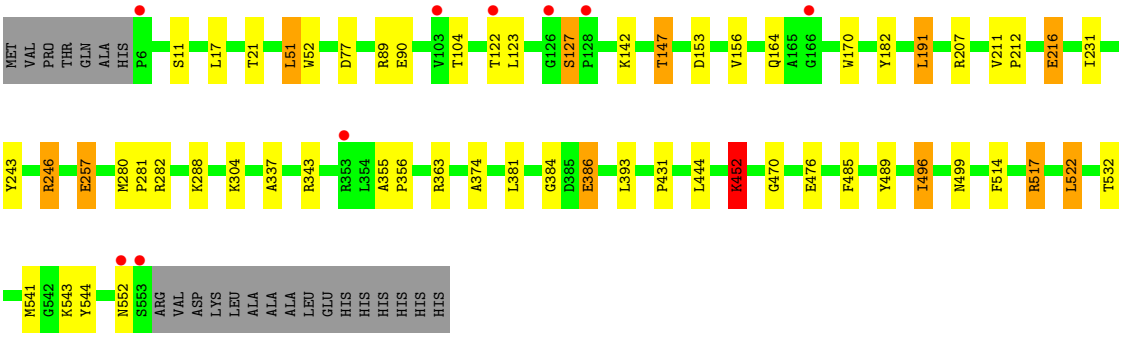
• Molecule 1: Trehalose synthase

Chain A:



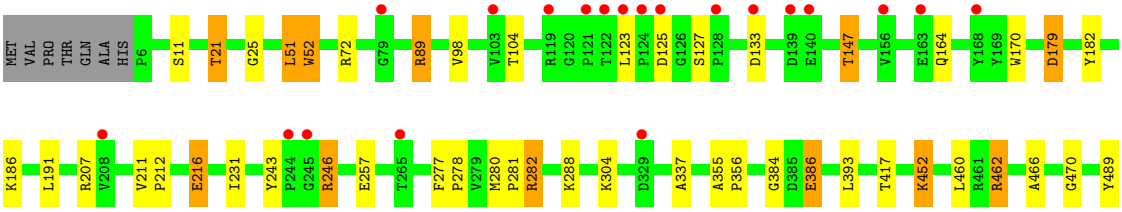
• Molecule 1: Trehalose synthase

Chain B:



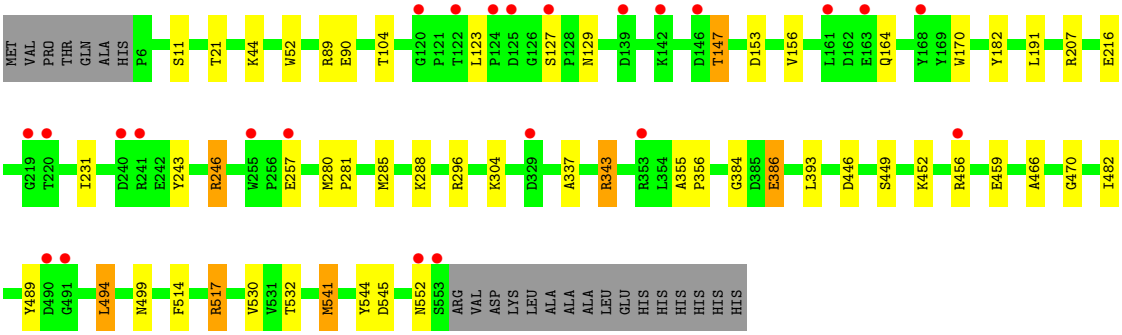
• Molecule 1: Trehalose synthase

Chain C:



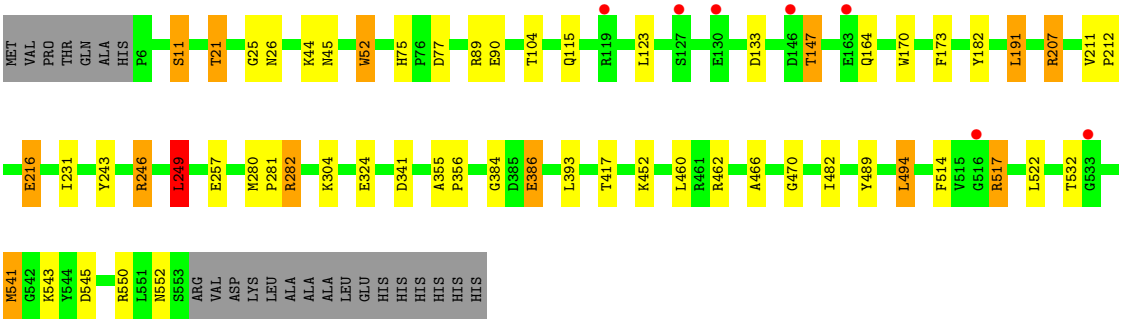
• Molecule 1: Trehalose synthase

Chain D:



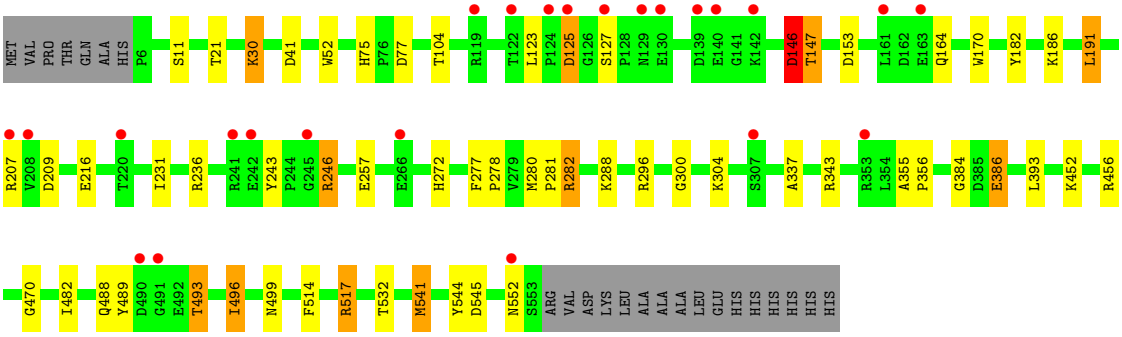
• Molecule 1: Trehalose synthase

Chain E:



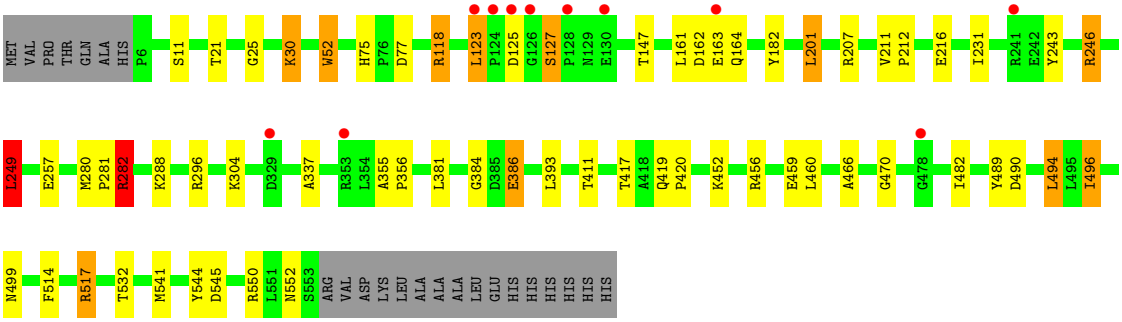
• Molecule 1: Trehalose synthase

Chain F:



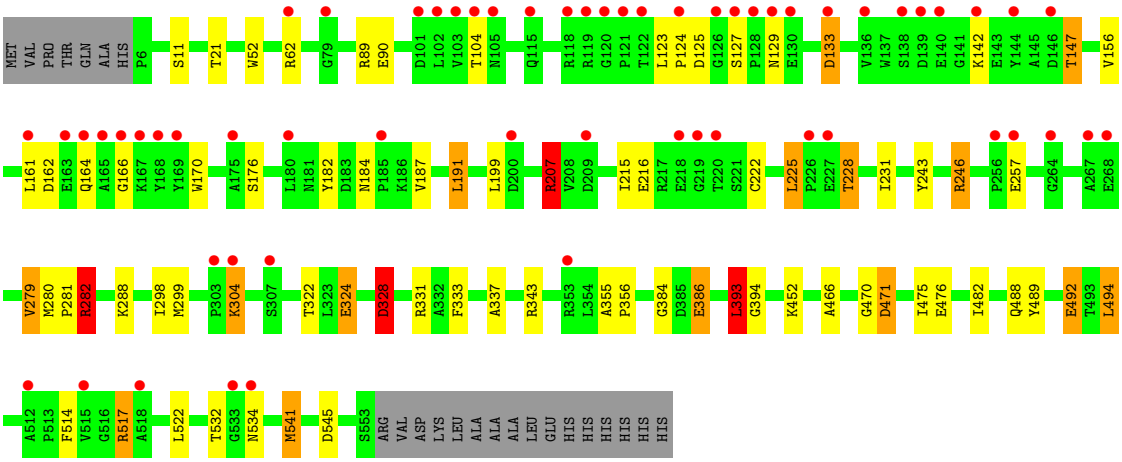
• Molecule 1: Trehalose synthase

Chain G:



- Molecule 1: Trehalose synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	95.61Å 195.90Å 130.99Å 90.00° 92.89° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.6 (30.00-2.70) 97.7 (29.96-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.194 , 0.236 0.197 , 0.239	Depositor DCC
R_{free} test set	6455 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.6	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36291	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, TRS

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	0.55	0/4537	0.77	8/6182 (0.1%)
1	B	0.55	0/4537	0.79	10/6182 (0.2%)
1	C	0.51	0/4537	0.74	6/6182 (0.1%)
1	D	0.50	0/4537	0.72	3/6182 (0.0%)
1	E	0.56	1/4537 (0.0%)	0.74	6/6182 (0.1%)
1	F	0.51	0/4537	0.74	5/6182 (0.1%)
1	G	0.53	0/4537	0.74	4/6182 (0.1%)
1	H	0.52	0/4537	0.79	11/6182 (0.2%)
All	All	0.53	1/36296 (0.0%)	0.75	53/49456 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	GLU	CD-OE2	-5.76	1.19	1.25

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	475	ILE	CG1-CB-CG2	-10.22	88.91	111.40
1	B	452	LYS	CD-CE-NZ	9.94	134.56	111.70
1	D	285	MET	CG-SD-CE	-9.54	84.94	100.20
1	F	146	ASP	CB-CG-OD2	8.68	126.11	118.30
1	E	543	LYS	CD-CE-NZ	8.36	130.94	111.70
1	A	17	LEU	CB-CG-CD2	8.29	125.10	111.00
1	F	41	ASP	CB-CG-OD1	-7.74	111.33	118.30
1	A	30	LYS	CD-CE-NZ	-7.71	93.97	111.70
1	B	522	LEU	CB-CG-CD2	7.67	124.03	111.00
1	D	343	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	C	541	MET	CG-SD-CE	7.59	112.35	100.20
1	C	522	LEU	CB-CG-CD2	7.38	123.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	THR	N-CA-CB	-7.35	96.34	110.30
1	A	541	MET	CG-SD-CE	7.33	111.92	100.20
1	E	249	LEU	CA-CB-CG	7.27	132.03	115.30
1	B	541	MET	CG-SD-CE	7.19	111.71	100.20
1	G	249	LEU	CA-CB-CG	7.12	131.67	115.30
1	G	490	ASP	CB-CA-C	7.06	124.52	110.40
1	F	41	ASP	CB-CG-OD2	7.00	124.60	118.30
1	H	207	ARG	CG-CD-NE	6.77	126.02	111.80
1	B	77	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	H	393	LEU	CB-CG-CD1	-6.50	99.96	111.00
1	C	452	LYS	CD-CE-NZ	6.26	126.09	111.70
1	E	462	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	78	LEU	CA-CB-CG	6.17	129.49	115.30
1	H	246	ARG	CA-CB-CG	-6.11	99.97	113.40
1	B	77	ASP	CB-CG-OD1	6.02	123.72	118.30
1	F	541	MET	CG-SD-CE	-5.95	90.68	100.20
1	E	541	MET	CG-SD-CE	-5.93	90.71	100.20
1	H	328	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	543	LYS	CD-CE-NZ	5.79	125.03	111.70
1	H	541	MET	CG-SD-CE	-5.79	90.94	100.20
1	B	363	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	51	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	543	LYS	CD-CE-NZ	5.59	124.57	111.70
1	H	279	VAL	CB-CA-C	-5.59	100.77	111.40
1	B	386	GLU	CG-CD-OE1	-5.55	107.20	118.30
1	H	328	ASP	N-CA-CB	5.54	120.57	110.60
1	G	282	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	17	LEU	CA-CB-CG	5.45	127.83	115.30
1	H	471	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	C	51	LEU	CA-CB-CG	5.31	127.50	115.30
1	B	51	LEU	CA-CB-CG	5.29	127.47	115.30
1	E	462	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	C	125	ASP	CB-CA-C	-5.23	99.94	110.40
1	H	246	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	216	GLU	CG-CD-OE2	5.11	128.51	118.30
1	E	207	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	F	496	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	G	496	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	D	541	MET	CG-SD-CE	-5.05	92.12	100.20
1	A	492	GLU	CG-CD-OE1	5.02	128.34	118.30
1	H	282	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4404	0	4201	35	0
1	B	4404	0	4201	29	0
1	C	4404	0	4201	37	0
1	D	4404	0	4201	39	0
1	E	4404	0	4201	43	0
1	F	4404	0	4201	40	0
1	G	4404	0	4201	43	0
1	H	4404	0	4201	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	12	1	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
4	E	8	0	12	1	0
4	F	8	0	12	0	0
4	G	8	0	12	0	0
4	H	8	0	12	0	0
5	A	157	0	0	1	0
5	B	147	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	107	0	0	4	0
5	D	99	0	0	3	0
5	E	193	0	0	6	0
5	F	85	0	0	1	0
5	G	133	0	0	1	0
5	H	58	0	0	6	0
All	All	36291	0	33704	291	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 4.

All (291) 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:D:182:TYR:OH	1:D:191:LEU:CD1	2.07	1.02
1:C:182:TYR:OH	1:C:191:LEU:CD1	2.08	1.01
1:G:118:ARG:NH1	1:G:162:ASP:OD2	2.01	0.93
1:B:123:LEU:HB2	5:B:819:HOH:O	1.71	0.87
1:D:182:TYR:OH	1:D:191:LEU:HD13	1.75	0.86
1:B:127:SER:N	5:B:819:HOH:O	2.08	0.85
1:H:125:ASP:HB2	5:H:718:HOH:O	1.76	0.85
1:D:52:TRP:CZ2	1:D:207:ARG:HD3	2.12	0.85
1:F:52:TRP:CZ2	1:F:207:ARG:HD3	2.10	0.85
1:C:182:TYR:OH	1:C:191:LEU:HD13	1.76	0.84
1:A:52:TRP:CZ2	1:A:207:ARG:HD3	2.11	0.84
1:G:52:TRP:CZ2	1:G:207:ARG:HD3	2.13	0.84
1:C:52:TRP:CZ2	1:C:207:ARG:HD3	2.14	0.83
1:E:52:TRP:CZ2	1:E:207:ARG:HD3	2.14	0.81
1:D:182:TYR:OH	1:D:191:LEU:HD11	1.80	0.81
1:C:182:TYR:OH	1:C:191:LEU:HD11	1.81	0.77
1:H:52:TRP:CZ2	1:H:207:ARG:HD3	2.20	0.76
1:H:482:ILE:HG23	1:H:541:MET:HE1	1.68	0.75
1:D:482:ILE:HG23	1:D:541:MET:HE1	1.67	0.74
1:C:179:ASP:HB3	5:C:807:HOH:O	1.87	0.74
1:C:216:GLU:OE1	5:C:807:HOH:O	2.05	0.73
1:E:482:ILE:HG23	1:E:541:MET:HE1	1.70	0.73
1:H:184:ASN:OD1	1:H:187:VAL:HG23	1.89	0.73
1:G:482:ILE:HG23	1:G:541:MET:HE1	1.71	0.73
1:B:374:ALA:CB	1:B:496:ILE:HD13	2.18	0.72
1:H:199:LEU:HD22	1:H:246:ARG:HD3	1.72	0.71
1:H:215:ILE:HB	1:H:228:THR:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:O	1:B:452:LYS:NZ	2.25	0.69
1:H:492:GLU:HA	1:H:492:GLU:OE1	1.93	0.69
1:E:216:GLU:HG2	5:E:745:HOH:O	1.94	0.68
1:F:482:ILE:HG23	1:F:541:MET:HE1	1.75	0.68
1:B:485:PHE:CZ	1:B:496:ILE:HG12	2.28	0.68
1:G:296:ARG:NH1	5:G:770:HOH:O	2.27	0.68
1:H:222:CYS:O	5:H:708:HOH:O	2.12	0.68
1:E:75:HIS:ND1	1:E:77:ASP:OD1	2.28	0.66
1:E:341:ASP:HB3	5:E:868:HOH:O	1.95	0.66
1:F:30:LYS:HE3	1:F:77:ASP:CB	2.24	0.66
1:F:125:ASP:OD1	1:F:125:ASP:O	2.15	0.65
1:H:133:ASP:OD1	1:H:133:ASP:N	2.29	0.65
1:H:328:ASP:OD1	1:H:331:ARG:NH1	2.30	0.65
1:A:288:LYS:HG3	1:A:337:ALA:HB1	1.78	0.65
1:G:30:LYS:HE3	1:G:77:ASP:CB	2.27	0.65
1:F:75:HIS:ND1	1:F:77:ASP:OD1	2.31	0.64
1:G:207:ARG:HG3	1:G:249:LEU:HD13	1.79	0.64
1:H:243:TYR:HB3	1:H:246:ARG:HD2	1.79	0.64
1:E:21:THR:HG22	5:E:725:HOH:O	1.97	0.63
1:E:207:ARG:HG3	1:E:249:LEU:HD13	1.81	0.63
1:G:75:HIS:ND1	1:G:77:ASP:OD1	2.32	0.62
1:A:74:ILE:HD11	1:A:79:GLY:O	2.00	0.62
1:C:545:ASP:OD2	1:D:545:ASP:OD2	2.18	0.61
1:H:282:ARG:HD3	1:H:282:ARG:N	2.15	0.61
1:F:236:ARG:CZ	1:F:272:HIS:CD2	2.84	0.61
1:G:118:ARG:NH1	1:G:162:ASP:CG	2.54	0.60
1:G:282:ARG:HD3	1:G:282:ARG:N	2.15	0.60
1:A:75:HIS:ND1	1:A:77:ASP:OD1	2.34	0.59
1:F:30:LYS:HE3	1:F:77:ASP:HB3	1.84	0.58
1:A:25:GLY:HA3	1:E:417:THR:HG21	1.85	0.58
1:A:280:MET:HB3	1:A:281:PRO:HD3	1.85	0.58
1:G:482:ILE:HG23	1:G:541:MET:CE	2.34	0.58
1:C:282:ARG:HD3	1:C:282:ARG:N	2.18	0.57
1:D:52:TRP:CE2	1:D:207:ARG:HD3	2.39	0.57
1:F:488:GLN:HG2	1:F:493:THR:HB	1.86	0.57
1:C:104:THR:HG22	1:C:191:LEU:HD22	1.87	0.57
1:E:482:ILE:HG23	1:E:541:MET:CE	2.34	0.57
1:H:333:PHE:CD1	1:H:333:PHE:C	2.78	0.57
1:H:225:LEU:HB2	1:H:228:THR:HG23	1.85	0.56
1:E:282:ARG:HD3	1:E:282:ARG:N	2.19	0.56
1:C:553:SER:O	1:H:156:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:ARG:HD3	1:F:282:ARG:N	2.20	0.56
1:H:482:ILE:HG23	1:H:541:MET:CE	2.35	0.56
1:G:52:TRP:CE2	1:G:207:ARG:HD3	2.40	0.56
1:C:417:THR:HG21	1:G:25:GLY:HA3	1.87	0.56
1:E:52:TRP:CE2	1:E:207:ARG:HD3	2.41	0.55
1:F:482:ILE:HG23	1:F:541:MET:CE	2.35	0.55
1:D:104:THR:HG22	1:D:191:LEU:HD22	1.88	0.55
1:B:431:PRO:HD3	1:E:45:ASN:ND2	2.21	0.55
1:H:123:LEU:HB3	1:H:124:PRO:HD2	1.88	0.55
1:C:72:ARG:NH1	5:C:711:HOH:O	2.40	0.55
1:G:30:LYS:HE3	1:G:77:ASP:HB3	1.89	0.55
1:D:343:ARG:NH2	1:G:459:GLU:OE1	2.30	0.55
1:D:343:ARG:NH2	1:G:459:GLU:HB3	2.22	0.55
1:F:52:TRP:CE2	1:F:207:ARG:HD3	2.40	0.54
1:B:374:ALA:HB1	1:B:496:ILE:HD13	1.88	0.54
1:F:280:MET:HB3	1:F:281:PRO:HD3	1.89	0.54
1:D:153:ASP:O	1:G:550:ARG:NH2	2.36	0.54
1:D:280:MET:HB3	1:D:281:PRO:HD3	1.89	0.54
1:C:52:TRP:CE2	1:C:207:ARG:HD3	2.41	0.54
1:D:456:ARG:NH1	5:D:795:HOH:O	2.38	0.54
1:D:482:ILE:HG23	1:D:541:MET:CE	2.34	0.54
1:H:534:ASN:HB3	5:H:734:HOH:O	2.07	0.54
1:H:280:MET:HB3	1:H:281:PRO:HD3	1.90	0.53
1:C:280:MET:HB3	1:C:281:PRO:HD3	1.90	0.53
1:B:280:MET:HB3	1:B:281:PRO:HD3	1.90	0.53
1:F:482:ILE:HG12	1:F:541:MET:HE1	1.90	0.53
1:A:52:TRP:CE2	1:A:207:ARG:HD3	2.42	0.53
1:G:280:MET:HB3	1:G:281:PRO:HD3	1.90	0.53
1:E:280:MET:HB3	1:E:281:PRO:HD3	1.91	0.53
1:H:222:CYS:HB3	5:H:708:HOH:O	2.09	0.53
1:G:470:GLY:HA2	1:G:489:TYR:HB2	1.91	0.52
1:H:222:CYS:HA	1:H:225:LEU:HD21	1.90	0.52
1:C:462:ARG:NH2	1:H:394:GLY:HA3	2.24	0.52
1:A:419:GLN:HG3	1:A:420:PRO:HD2	1.91	0.52
1:E:470:GLY:HA2	1:E:489:TYR:HB2	1.92	0.52
1:D:470:GLY:HA2	1:D:489:TYR:HB2	1.92	0.51
1:E:466:ALA:HB3	1:E:494:LEU:HD22	1.92	0.51
1:D:123:LEU:HD21	1:D:129:ASN:HD22	1.76	0.51
1:G:419:GLN:HG3	1:G:420:PRO:HD2	1.92	0.51
1:H:162:ASP:HB3	5:H:714:HOH:O	2.11	0.50
1:H:470:GLY:HA2	1:H:489:TYR:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:ILE:HG12	1:H:541:MET:CE	2.41	0.50
1:F:482:ILE:HG12	1:F:541:MET:CE	2.42	0.50
1:F:236:ARG:CZ	1:F:272:HIS:HD2	2.25	0.50
1:A:74:ILE:HD11	1:A:79:GLY:C	2.32	0.50
1:C:470:GLY:HA2	1:C:489:TYR:HB2	1.93	0.50
1:G:545:ASP:OD2	1:H:545:ASP:OD2	2.30	0.50
1:H:355:ALA:HB3	1:H:356:PRO:HD3	1.94	0.50
1:F:470:GLY:HA2	1:F:489:TYR:HB2	1.94	0.50
1:G:482:ILE:HG12	1:G:541:MET:CE	2.42	0.50
1:C:182:TYR:HB3	1:C:231:ILE:CD1	2.42	0.50
1:F:123:LEU:C	1:F:125:ASP:H	2.15	0.50
1:B:470:GLY:HA2	1:B:489:TYR:HB2	1.93	0.49
1:E:482:ILE:HG12	1:E:541:MET:CE	2.42	0.49
1:D:482:ILE:CG2	1:D:541:MET:HE1	2.41	0.49
1:F:30:LYS:HE3	1:F:77:ASP:HB2	1.93	0.49
1:C:466:ALA:HB3	1:C:494:LEU:HD22	1.95	0.49
1:E:482:ILE:HG12	1:E:541:MET:HE1	1.94	0.49
1:H:279:VAL:CG1	1:H:299:MET:SD	3.01	0.49
1:A:470:GLY:HA2	1:A:489:TYR:HB2	1.94	0.49
1:B:182:TYR:HB3	1:B:231:ILE:CD1	2.43	0.49
1:H:182:TYR:HB3	1:H:231:ILE:CD1	2.42	0.49
1:H:343:ARG:NH2	1:H:393:LEU:O	2.39	0.49
1:H:482:ILE:CG2	1:H:541:MET:HE1	2.41	0.49
1:H:322:THR:OG1	1:H:324:GLU:CG	2.61	0.49
1:C:460:LEU:HD13	1:H:343:ARG:CD	2.43	0.48
1:D:482:ILE:HG12	1:D:541:MET:CE	2.42	0.48
1:G:482:ILE:HG12	1:G:541:MET:HE1	1.95	0.48
1:D:89:ARG:NH1	1:D:90:GLU:OE1	2.47	0.48
1:D:296:ARG:HD3	5:D:719:HOH:O	2.12	0.48
1:F:182:TYR:HB3	1:F:231:ILE:CD1	2.43	0.48
1:E:355:ALA:HB3	1:E:356:PRO:HD3	1.96	0.48
1:F:243:TYR:HB3	1:F:246:ARG:HG2	1.95	0.48
1:H:466:ALA:HB3	1:H:494:LEU:HD22	1.95	0.48
1:B:153:ASP:O	1:E:550:ARG:NH2	2.39	0.48
1:C:460:LEU:HD13	1:H:343:ARG:HD2	1.95	0.48
1:E:182:TYR:HB3	1:E:231:ILE:CD1	2.43	0.48
1:G:466:ALA:HB3	1:G:494:LEU:HD22	1.94	0.48
1:G:30:LYS:HE3	1:G:77:ASP:HB2	1.95	0.48
1:G:482:ILE:CG2	1:G:541:MET:CE	2.92	0.48
1:E:243:TYR:HB3	1:E:246:ARG:HG2	1.96	0.48
1:E:173:PHE:CE1	4:E:602:TRS:H12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TYR:HB3	1:A:231:ILE:CD1	2.43	0.47
1:B:243:TYR:HB3	1:B:246:ARG:HG2	1.95	0.47
1:G:118:ARG:NH1	1:G:162:ASP:OD1	2.47	0.47
1:H:215:ILE:H	1:H:228:THR:HG22	1.79	0.47
1:F:355:ALA:HB3	1:F:356:PRO:HD3	1.97	0.47
1:H:279:VAL:HG11	1:H:299:MET:SD	2.54	0.47
1:A:81:LEU:O	1:A:81:LEU:HD22	2.15	0.47
1:D:182:TYR:HB3	1:D:231:ILE:CD1	2.44	0.47
1:D:243:TYR:HB3	1:D:246:ARG:HG2	1.96	0.47
1:D:466:ALA:HB3	1:D:494:LEU:HD22	1.96	0.47
1:E:482:ILE:CG2	1:E:541:MET:CE	2.92	0.47
1:G:182:TYR:HB3	1:G:231:ILE:CD1	2.45	0.47
1:G:243:TYR:HB3	1:G:246:ARG:HG2	1.97	0.47
1:G:355:ALA:HB3	1:G:356:PRO:HD3	1.96	0.47
1:H:104:THR:HG22	1:H:191:LEU:CD2	2.45	0.47
1:H:104:THR:HG22	1:H:191:LEU:HD22	1.97	0.47
1:A:104:THR:HG22	1:A:191:LEU:CD2	2.45	0.47
1:C:25:GLY:HA3	1:G:417:THR:HG21	1.97	0.47
1:A:75:HIS:HB3	1:A:78:LEU:HD22	1.97	0.47
1:A:104:THR:HG22	1:A:191:LEU:HD22	1.97	0.47
1:C:417:THR:HG21	1:G:25:GLY:CA	2.45	0.46
1:D:482:ILE:CG2	1:D:541:MET:CE	2.93	0.46
1:B:355:ALA:HB3	1:B:356:PRO:HD3	1.95	0.46
1:C:21:THR:HG22	5:C:720:HOH:O	2.14	0.46
1:C:243:TYR:HB3	1:C:246:ARG:HG2	1.96	0.46
1:F:104:THR:HG22	1:F:191:LEU:CD2	2.46	0.46
1:H:482:ILE:HG12	1:H:541:MET:HE1	1.98	0.46
1:A:355:ALA:HB3	1:A:356:PRO:HD3	1.98	0.46
1:A:384:GLY:N	1:A:386:GLU:OE2	2.48	0.46
1:H:482:ILE:CG2	1:H:541:MET:CE	2.93	0.46
1:C:460:LEU:HD13	1:H:343:ARG:NE	2.31	0.46
1:E:45:ASN:HB3	5:E:832:HOH:O	2.15	0.46
1:A:243:TYR:HB3	1:A:246:ARG:HG2	1.96	0.46
1:B:89:ARG:NH1	1:B:90:GLU:OE1	2.48	0.46
1:E:384:GLY:N	1:E:386:GLU:OE2	2.49	0.46
1:C:355:ALA:HB3	1:C:356:PRO:HD3	1.98	0.45
1:D:384:GLY:N	1:D:386:GLU:OE2	2.49	0.45
1:E:89:ARG:NH1	1:E:90:GLU:OE1	2.48	0.45
1:H:166:GLY:N	5:H:714:HOH:O	2.49	0.45
1:H:384:GLY:N	1:H:386:GLU:OE2	2.49	0.45
1:A:289:ARG:HG3	1:A:333:PHE:CZ	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:104:THR:HG22	1:F:191:LEU:HD22	1.98	0.45
1:H:123:LEU:HD11	1:H:129:ASN:HA	1.97	0.45
1:H:304:LYS:H	1:H:304:LYS:HD2	1.81	0.45
1:A:26:ASN:C	1:E:26:ASN:HA	2.37	0.45
1:D:288:LYS:HG3	1:D:337:ALA:HB1	1.99	0.45
1:E:104:THR:HG22	1:E:191:LEU:CD2	2.47	0.45
1:E:545:ASP:OD2	1:F:545:ASP:OD2	2.34	0.45
1:F:482:ILE:CG2	1:F:541:MET:CE	2.94	0.45
1:B:104:THR:HG22	1:B:191:LEU:HD22	1.98	0.45
1:D:156:VAL:HG13	1:G:552:ASN:HB3	1.98	0.45
1:H:89:ARG:NH1	1:H:90:GLU:OE1	2.49	0.45
1:B:170:TRP:NE1	1:B:216:GLU:HG2	2.31	0.45
1:H:322:THR:OG1	1:H:324:GLU:HG2	2.17	0.45
1:D:355:ALA:HB3	1:D:356:PRO:HD3	1.99	0.45
1:E:104:THR:HG22	1:E:191:LEU:HD22	1.98	0.45
1:B:104:THR:HG22	1:B:191:LEU:CD2	2.46	0.44
1:H:62:ARG:HE	1:H:176:SER:CB	2.30	0.44
1:B:156:VAL:HG13	1:E:552:ASN:HB3	1.99	0.44
1:E:115:GLN:HG3	5:E:801:HOH:O	2.16	0.44
1:B:343:ARG:HD3	1:E:460:LEU:HD13	1.99	0.44
1:F:384:GLY:N	1:F:386:GLU:OE2	2.49	0.44
1:G:482:ILE:CG2	1:G:541:MET:HE1	2.43	0.44
1:A:25:GLY:CA	1:E:417:THR:HG21	2.47	0.44
1:A:460:LEU:HD13	1:F:343:ARG:HD3	2.00	0.44
1:D:499:ASN:O	1:D:544:TYR:HA	2.18	0.44
1:F:482:ILE:CG2	1:F:541:MET:HE1	2.46	0.44
1:F:246:ARG:N	1:F:246:ARG:HD3	2.33	0.43
1:G:384:GLY:N	1:G:386:GLU:OE2	2.50	0.43
1:A:66:TYR:CD1	4:A:602:TRS:H31	2.53	0.43
1:B:17:LEU:C	1:B:17:LEU:HD12	2.38	0.43
1:B:288:LYS:HG3	1:B:337:ALA:HB1	2.00	0.43
1:E:514:PHE:HB3	1:E:517:ARG:HG3	1.99	0.43
1:A:417:THR:HG21	1:E:25:GLY:HA3	1.99	0.43
1:D:343:ARG:NH1	1:G:456:ARG:HG3	2.33	0.43
1:D:530:VAL:HG23	5:D:706:HOH:O	2.18	0.43
1:D:246:ARG:HD3	1:D:246:ARG:N	2.34	0.43
1:F:517:ARG:HB3	1:F:552:ASN:O	2.19	0.43
1:H:147:THR:HG21	1:H:170:TRP:HH2	1.84	0.43
1:D:343:ARG:HD2	1:G:460:LEU:HD13	2.00	0.43
1:C:288:LYS:HG3	1:C:337:ALA:HB1	2.01	0.42
1:A:147:THR:HG23	1:A:158:ASN:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:THR:HG21	1:E:170:TRP:HH2	1.84	0.42
1:B:517:ARG:HB3	1:B:552:ASN:O	2.19	0.42
1:E:482:ILE:CG2	1:E:541:MET:HE1	2.42	0.42
1:H:222:CYS:HA	1:H:225:LEU:CD2	2.49	0.42
1:H:288:LYS:HG3	1:H:337:ALA:HB1	2.02	0.42
1:A:246:ARG:N	1:A:246:ARG:HD3	2.34	0.42
1:H:514:PHE:HB3	1:H:517:ARG:HG3	2.00	0.42
1:B:499:ASN:O	1:B:544:TYR:HA	2.20	0.42
1:C:384:GLY:N	1:C:386:GLU:OE2	2.49	0.42
1:C:514:PHE:HB3	1:C:517:ARG:HG3	2.01	0.42
1:D:482:ILE:HG12	1:D:541:MET:HE1	2.00	0.42
1:B:147:THR:HG21	1:B:170:TRP:HH2	1.84	0.41
1:G:123:LEU:HD23	1:G:127:SER:HB2	2.01	0.41
1:A:20:ARG:HD2	1:A:424:PHE:CE2	2.55	0.41
1:F:125:ASP:OD1	1:F:125:ASP:C	2.59	0.41
1:C:211:VAL:N	1:C:212:PRO:CD	2.83	0.41
1:E:11:SER:OG	5:E:865:HOH:O	2.11	0.41
1:C:553:SER:O	1:H:156:VAL:CG2	2.69	0.41
1:F:277:PHE:N	1:F:278:PRO:CD	2.83	0.41
1:G:499:ASN:O	1:G:544:TYR:HA	2.20	0.41
1:D:123:LEU:HD21	1:D:129:ASN:ND2	2.36	0.41
1:F:300:GLY:C	5:F:701:HOH:O	2.57	0.41
1:G:288:LYS:HG3	1:G:337:ALA:HB1	2.02	0.41
1:A:550:ARG:NH2	1:F:153:ASP:O	2.49	0.41
1:C:147:THR:HG21	1:C:170:TRP:HH2	1.86	0.41
1:D:517:ARG:HB3	1:D:552:ASN:O	2.20	0.41
1:C:517:ARG:HB3	1:C:552:ASN:O	2.21	0.41
1:D:147:THR:HG21	1:D:170:TRP:HH2	1.85	0.41
1:G:201:LEU:HA	1:G:201:LEU:HD12	1.81	0.41
1:A:26:ASN:HA	1:E:26:ASN:C	2.41	0.41
1:A:52:TRP:CD1	1:A:52:TRP:C	2.93	0.41
1:A:277:PHE:N	1:A:278:PRO:CD	2.83	0.41
1:A:288:LYS:CG	1:A:337:ALA:HB1	2.49	0.41
1:F:147:THR:HG21	1:F:170:TRP:HH2	1.86	0.41
1:F:207:ARG:NH2	1:F:209:ASP:OD2	2.54	0.41
1:F:288:LYS:HG3	1:F:337:ALA:HB1	2.02	0.41
1:G:125:ASP:OD1	1:G:127:SER:OG	2.39	0.41
1:G:514:PHE:HB3	1:G:517:ARG:HG3	2.02	0.41
1:A:123:LEU:HD23	1:A:127:SER:HB2	2.01	0.41
1:B:257:GLU:CD	1:B:257:GLU:H	2.25	0.41
1:C:246:ARG:N	1:C:246:ARG:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:PHE:N	1:C:278:PRO:CD	2.84	0.41
1:E:211:VAL:N	1:E:212:PRO:CD	2.84	0.41
1:F:499:ASN:O	1:F:544:TYR:HA	2.20	0.41
1:G:211:VAL:N	1:G:212:PRO:CD	2.84	0.41
1:A:514:PHE:HB3	1:A:517:ARG:HG3	2.02	0.40
1:E:517:ARG:HB3	1:E:552:ASN:O	2.21	0.40
1:A:293:SER:HB3	5:A:820:HOH:O	2.22	0.40
1:C:499:ASN:O	1:C:544:TYR:HA	2.21	0.40
1:F:146:ASP:OD1	1:F:146:ASP:N	2.53	0.40
1:B:52:TRP:CD1	1:B:52:TRP:C	2.95	0.40
1:C:89:ARG:NE	1:C:89:ARG:HA	2.37	0.40
1:D:514:PHE:HB3	1:D:517:ARG:HG3	2.02	0.40
1:F:514:PHE:HB3	1:F:517:ARG:HG3	2.03	0.40
1:B:384:GLY:N	1:B:386:GLU:OE2	2.52	0.40
1:D:446:ASP:HB3	1:D:449:SER:HB3	2.04	0.40
1:E:246:ARG:N	1:E:246:ARG:HD3	2.35	0.40
1:B:211:VAL:N	1:B:212:PRO:CD	2.84	0.40
1:B:514:PHE:HB3	1:B:517:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/571 (96%)	532 (97%)	14 (3%)	0	100	100
1	B	546/571 (96%)	532 (97%)	14 (3%)	0	100	100
1	C	546/571 (96%)	531 (97%)	15 (3%)	0	100	100
1	D	546/571 (96%)	532 (97%)	14 (3%)	0	100	100
1	E	546/571 (96%)	531 (97%)	15 (3%)	0	100	100
1	F	546/571 (96%)	530 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	546/571 (96%)	533 (98%)	13 (2%)	0	100	100
1	H	546/571 (96%)	533 (98%)	13 (2%)	0	100	100
All	All	4368/4568 (96%)	4254 (97%)	114 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	465/484 (96%)	434 (93%)	31 (7%)	16	37
1	B	465/484 (96%)	443 (95%)	22 (5%)	26	54
1	C	465/484 (96%)	439 (94%)	26 (6%)	21	45
1	D	465/484 (96%)	448 (96%)	17 (4%)	34	63
1	E	465/484 (96%)	443 (95%)	22 (5%)	26	54
1	F	465/484 (96%)	441 (95%)	24 (5%)	23	49
1	G	465/484 (96%)	438 (94%)	27 (6%)	20	43
1	H	465/484 (96%)	435 (94%)	30 (6%)	17	38
All	All	3720/3872 (96%)	3521 (95%)	199 (5%)	22	48

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	17	LEU
1	A	21	THR
1	A	30	LYS
1	A	51	LEU
1	A	68	VAL
1	A	74	ILE
1	A	78	LEU
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	98	VAL
1	A	123	LEU
1	A	127	SER
1	A	133	ASP
1	A	147	THR
1	A	152	THR
1	A	161	LEU
1	A	164	GLN
1	A	186	LYS
1	A	191	LEU
1	A	216	GLU
1	A	246	ARG
1	A	257	GLU
1	A	282	ARG
1	A	288	LYS
1	A	304	LYS
1	A	381	LEU
1	A	386	GLU
1	A	393	LEU
1	A	452	LYS
1	A	517	ARG
1	A	532	THR
1	B	11	SER
1	B	21	THR
1	B	51	LEU
1	B	122	THR
1	B	127	SER
1	B	142	LYS
1	B	147	THR
1	B	164	GLN
1	B	191	LEU
1	B	207	ARG
1	B	246	ARG
1	B	257	GLU
1	B	282	ARG
1	B	304	LYS
1	B	381	LEU
1	B	393	LEU
1	B	452	LYS
1	B	476	GLU
1	B	496	ILE
1	B	517	ARG

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Mol	Chain	Res	Type
1	B	522	LEU
1	B	532	THR
1	C	11	SER
1	C	21	THR
1	C	51	LEU
1	C	52	TRP
1	C	89	ARG
1	C	98	VAL
1	C	123	LEU
1	C	127	SER
1	C	133	ASP
1	C	147	THR
1	C	164	GLN
1	C	179	ASP
1	C	186	LYS
1	C	216	GLU
1	C	246	ARG
1	C	257	GLU
1	C	282	ARG
1	C	304	LYS
1	C	386	GLU
1	C	393	LEU
1	C	452	LYS
1	C	462	ARG
1	C	494	LEU
1	C	517	ARG
1	C	522	LEU
1	C	532	THR
1	D	11	SER
1	D	21	THR
1	D	44	LYS
1	D	127	SER
1	D	147	THR
1	D	164	GLN
1	D	216	GLU
1	D	246	ARG
1	D	257	GLU
1	D	304	LYS
1	D	386	GLU
1	D	393	LEU
1	D	452	LYS
1	D	459	GLU

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Mol	Chain	Res	Type
1	D	494	LEU
1	D	517	ARG
1	D	532	THR
1	E	11	SER
1	E	21	THR
1	E	44	LYS
1	E	52	TRP
1	E	123	LEU
1	E	133	ASP
1	E	147	THR
1	E	164	GLN
1	E	191	LEU
1	E	216	GLU
1	E	246	ARG
1	E	249	LEU
1	E	257	GLU
1	E	282	ARG
1	E	304	LYS
1	E	386	GLU
1	E	393	LEU
1	E	452	LYS
1	E	494	LEU
1	E	517	ARG
1	E	522	LEU
1	E	532	THR
1	F	11	SER
1	F	21	THR
1	F	30	LYS
1	F	125	ASP
1	F	127	SER
1	F	146	ASP
1	F	147	THR
1	F	164	GLN
1	F	186	LYS
1	F	191	LEU
1	F	216	GLU
1	F	246	ARG
1	F	257	GLU
1	F	282	ARG
1	F	296	ARG
1	F	304	LYS
1	F	386	GLU

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Mol	Chain	Res	Type
1	F	393	LEU
1	F	452	LYS
1	F	456	ARG
1	F	493	THR
1	F	496	ILE
1	F	517	ARG
1	F	532	THR
1	G	11	SER
1	G	21	THR
1	G	30	LYS
1	G	52	TRP
1	G	118	ARG
1	G	123	LEU
1	G	127	SER
1	G	147	THR
1	G	161	LEU
1	G	163	GLU
1	G	164	GLN
1	G	201	LEU
1	G	216	GLU
1	G	246	ARG
1	G	249	LEU
1	G	257	GLU
1	G	282	ARG
1	G	304	LYS
1	G	381	LEU
1	G	386	GLU
1	G	393	LEU
1	G	411	THR
1	G	452	LYS
1	G	494	LEU
1	G	496	ILE
1	G	517	ARG
1	G	532	THR
1	H	11	SER
1	H	21	THR
1	H	127	SER
1	H	133	ASP
1	H	142	LYS
1	H	147	THR
1	H	161	LEU
1	H	164	GLN

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Mol	Chain	Res	Type
1	H	191	LEU
1	H	207	ARG
1	H	216	GLU
1	H	225	LEU
1	H	228	THR
1	H	257	GLU
1	H	282	ARG
1	H	298	ILE
1	H	304	LYS
1	H	324	GLU
1	H	328	ASP
1	H	386	GLU
1	H	393	LEU
1	H	452	LYS
1	H	471	ASP
1	H	476	GLU
1	H	488	GLN
1	H	492	GLU
1	H	494	LEU
1	H	517	ARG
1	H	522	LEU
1	H	532	THR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	TRS	C	602	-	7,7,7	0.61	0	9,9,9	0.75	0
4	TRS	F	602	-	7,7,7	0.46	0	9,9,9	0.80	0
4	TRS	D	602	-	7,7,7	0.34	0	9,9,9	0.58	0
4	TRS	E	602	-	7,7,7	0.52	0	9,9,9	0.70	0
4	TRS	B	602	-	7,7,7	0.49	0	9,9,9	1.15	0
4	TRS	A	602	-	7,7,7	0.56	0	9,9,9	0.73	0
4	TRS	H	602	-	7,7,7	0.33	0	9,9,9	0.65	0
4	TRS	G	602	-	7,7,7	0.38	0	9,9,9	0.86	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
4	TRS	C	602	-	-	6/9/9/9	-
4	TRS	F	602	-	-	6/9/9/9	-
4	TRS	D	602	-	-	6/9/9/9	-
4	TRS	E	602	-	-	6/9/9/9	-
4	TRS	B	602	-	-	9/9/9/9	-
4	TRS	A	602	-	-	6/9/9/9	-
4	TRS	H	602	-	-	5/9/9/9	-
4	TRS	G	602	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	TRS	C2-C-C1-O1
4	A	602	TRS	C3-C-C1-O1
4	B	602	TRS	C2-C-C1-O1
4	B	602	TRS	C3-C-C1-O1
4	B	602	TRS	C1-C-C2-O2
4	B	602	TRS	C3-C-C2-O2
4	C	602	TRS	C2-C-C1-O1
4	C	602	TRS	C3-C-C1-O1
4	C	602	TRS	N-C-C1-O1
4	D	602	TRS	C3-C-C1-O1
4	F	602	TRS	C3-C-C1-O1
4	F	602	TRS	C1-C-C3-O3
4	F	602	TRS	C2-C-C3-O3
4	F	602	TRS	N-C-C3-O3
4	H	602	TRS	N-C-C2-O2
4	H	602	TRS	N-C-C3-O3
4	A	602	TRS	C1-C-C3-O3
4	D	602	TRS	C2-C-C1-O1
4	F	602	TRS	C2-C-C1-O1
4	H	602	TRS	C3-C-C2-O2
4	H	602	TRS	C1-C-C3-O3
4	A	602	TRS	N-C-C1-O1
4	A	602	TRS	N-C-C3-O3
4	B	602	TRS	N-C-C2-O2
4	B	602	TRS	N-C-C3-O3
4	C	602	TRS	C2-C-C3-O3
4	C	602	TRS	N-C-C3-O3
4	D	602	TRS	N-C-C2-O2
4	E	602	TRS	N-C-C1-O1
4	E	602	TRS	C1-C-C2-O2
4	A	602	TRS	C2-C-C3-O3
4	B	602	TRS	C1-C-C3-O3
4	B	602	TRS	C2-C-C3-O3
4	C	602	TRS	C1-C-C3-O3
4	D	602	TRS	C1-C-C2-O2
4	E	602	TRS	C2-C-C1-O1
4	E	602	TRS	C3-C-C1-O1
4	E	602	TRS	C3-C-C2-O2
4	H	602	TRS	C1-C-C2-O2
4	B	602	TRS	N-C-C1-O1
4	D	602	TRS	N-C-C1-O1
4	D	602	TRS	C3-C-C2-O2
4	E	602	TRS	N-C-C2-O2

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Mol	Chain	Res	Type	Atoms
4	F	602	TRS	N-C-C1-O1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	602	TRS	1	0
4	A	602	TRS	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	548/571 (95%)	-0.31	3 (0%)	91	92	12, 28, 47, 80	3 (0%)
1	B	548/571 (95%)	-0.24	9 (1%)	72	74	13, 30, 54, 85	3 (0%)
1	C	548/571 (95%)	0.12	24 (4%)	34	33	16, 40, 64, 85	3 (0%)
1	D	548/571 (95%)	0.05	24 (4%)	34	33	14, 41, 71, 99	3 (0%)
1	E	548/571 (95%)	-0.43	7 (1%)	77	78	12, 25, 42, 84	3 (0%)
1	F	548/571 (95%)	0.10	24 (4%)	34	33	15, 38, 66, 110	3 (0%)
1	G	548/571 (95%)	-0.14	11 (2%)	65	67	19, 34, 57, 115	3 (0%)
1	H	548/571 (95%)	0.52	59 (10%)	5	4	23, 50, 84, 151	3 (0%)
All	All	4384/4568 (95%)	-0.04	161 (3%)	41	41	12, 35, 68, 151	24 (0%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	128	PRO	9.5
1	H	103	VAL	5.7
1	F	124	PRO	5.6
1	G	124	PRO	5.0
1	D	124	PRO	4.7
1	H	120	GLY	4.6
1	H	130	GLU	4.5
1	H	129	ASN	4.4
1	H	127	SER	4.3
1	C	119	ARG	4.2
1	H	121	PRO	4.1
1	H	180	LEU	4.0
1	F	163	GLU	3.9
1	H	163	GLU	3.9
1	H	220	THR	3.9
1	D	120	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	125	ASP	3.8
1	G	163	GLU	3.7
1	F	220	THR	3.7
1	C	128	PRO	3.6
1	F	127	SER	3.6
1	H	534	ASN	3.6
1	H	124	PRO	3.6
1	D	146	ASP	3.5
1	H	257	GLU	3.5
1	B	6	PRO	3.4
1	C	123	LEU	3.4
1	H	168	TYR	3.4
1	H	164	GLN	3.4
1	C	122	THR	3.3
1	H	227	GLU	3.3
1	H	219	GLY	3.2
1	H	139	ASP	3.2
1	H	146	ASP	3.2
1	F	122	THR	3.1
1	H	133	ASP	3.1
1	H	126	GLY	3.1
1	E	119	ARG	3.1
1	E	533	GLY	3.1
1	F	245	GLY	3.1
1	D	552	ASN	3.1
1	H	165	ALA	3.1
1	G	123	LEU	3.0
1	D	241	ARG	3.0
1	D	168	TYR	3.0
1	H	209	ASP	3.0
1	C	133	ASP	3.0
1	C	124	PRO	3.0
1	C	156	VAL	3.0
1	H	105	ASN	3.0
1	H	166	GLY	3.0
1	D	142	LYS	2.9
1	A	163	GLU	2.9
1	F	241	ARG	2.9
1	H	161	LEU	2.8
1	A	124	PRO	2.8
1	H	175	ALA	2.8
1	H	118	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	139	ASP	2.7
1	H	142	LYS	2.7
1	H	102	LEU	2.7
1	H	304	LYS	2.7
1	C	121	PRO	2.7
1	F	307	SER	2.7
1	G	128	PRO	2.7
1	H	256	PRO	2.7
1	B	353	ARG	2.7
1	D	240	ASP	2.7
1	H	267	ALA	2.6
1	B	553	SER	2.6
1	B	122	THR	2.6
1	H	303	PRO	2.6
1	D	257	GLU	2.6
1	F	142	LYS	2.6
1	D	161	LEU	2.6
1	H	169	TYR	2.6
1	D	163	GLU	2.6
1	F	552	ASN	2.6
1	C	125	ASP	2.6
1	H	200	ASP	2.6
1	H	167	LYS	2.6
1	A	145	ALA	2.5
1	F	139	ASP	2.5
1	C	516	GLY	2.5
1	E	127	SER	2.5
1	C	265	THR	2.5
1	G	126	GLY	2.5
1	H	122	THR	2.5
1	H	268	GLU	2.5
1	E	163	GLU	2.5
1	F	161	LEU	2.5
1	C	245	GLY	2.5
1	D	220	THR	2.5
1	H	119	ARG	2.5
1	B	128	PRO	2.4
1	D	122	THR	2.4
1	G	125	ASP	2.4
1	H	512	ALA	2.4
1	C	139	ASP	2.4
1	H	226	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	140	GLU	2.4
1	C	140	GLU	2.4
1	D	219	GLY	2.4
1	F	353	ARG	2.4
1	C	163	GLU	2.3
1	F	125	ASP	2.3
1	F	490	ASP	2.3
1	D	127	SER	2.3
1	C	208	VAL	2.3
1	D	255	TRP	2.3
1	H	515	VAL	2.3
1	H	101	ASP	2.3
1	C	103	VAL	2.3
1	E	146	ASP	2.3
1	H	533	GLY	2.2
1	G	130	GLU	2.2
1	D	491	GLY	2.2
1	H	104	THR	2.2
1	H	218	GLU	2.2
1	H	138	SER	2.2
1	H	62	ARG	2.2
1	F	208	VAL	2.2
1	C	532	THR	2.2
1	C	329	ASP	2.2
1	H	264	GLY	2.2
1	D	329	ASP	2.2
1	F	491	GLY	2.2
1	C	553	SER	2.1
1	B	126	GLY	2.1
1	H	79	GLY	2.1
1	H	353	ARG	2.1
1	C	168	TYR	2.1
1	H	307	SER	2.1
1	E	130	GLU	2.1
1	F	266	GLU	2.1
1	D	490	ASP	2.1
1	F	207	ARG	2.1
1	G	353	ARG	2.1
1	H	518	ALA	2.1
1	B	103	VAL	2.1
1	C	534	ASN	2.1
1	F	129	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	140	GLU	2.1
1	H	185	PRO	2.1
1	G	241	ARG	2.1
1	F	130	GLU	2.1
1	B	166	GLY	2.1
1	F	242	GLU	2.1
1	G	329	ASP	2.1
1	G	478	GLY	2.1
1	B	552	ASN	2.1
1	F	119	ARG	2.1
1	D	553	SER	2.1
1	E	516	GLY	2.1
1	H	144	TYR	2.0
1	C	244	PRO	2.0
1	D	456	ARG	2.0
1	C	79	GLY	2.0
1	D	353	ARG	2.0
1	H	136	VAL	2.0
1	H	115	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	CA	H	600	1/1	0.85	0.20	67,67,67,67	0
4	TRS	A	602	8/8	0.88	0.30	29,31,34,41	0
4	TRS	H	602	8/8	0.88	0.31	48,52,52,54	0
4	TRS	B	602	8/8	0.92	0.24	24,26,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	601	1/1	0.92	0.05	20,20,20,20	0
3	MG	G	601	1/1	0.93	0.09	16,16,16,16	0
3	MG	H	601	1/1	0.94	0.08	28,28,28,28	0
4	TRS	F	602	8/8	0.94	0.29	29,32,33,33	0
3	MG	E	601	1/1	0.94	0.11	7,7,7,7	0
4	TRS	C	602	8/8	0.95	0.20	27,29,30,32	0
4	TRS	D	602	8/8	0.95	0.27	34,34,35,35	0
4	TRS	E	602	8/8	0.95	0.19	21,21,22,22	0
2	CA	F	600	1/1	0.95	0.14	39,39,39,39	0
4	TRS	G	602	8/8	0.95	0.27	28,31,32,33	0
3	MG	B	601	1/1	0.95	0.10	8,8,8,8	0
2	CA	B	600	1/1	0.96	0.12	36,36,36,36	0
3	MG	A	601	1/1	0.96	0.14	14,14,14,14	0
2	CA	D	600	1/1	0.96	0.11	44,44,44,44	0
2	CA	A	600	1/1	0.96	0.06	32,32,32,32	0
2	CA	G	600	1/1	0.96	0.08	30,30,30,30	0
2	CA	E	600	1/1	0.97	0.10	25,25,25,25	0
2	CA	C	600	1/1	0.98	0.12	38,38,38,38	0
3	MG	C	601	1/1	0.99	0.05	12,12,12,12	0
3	MG	D	601	1/1	0.99	0.06	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.