



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:51 PM GMT

PDB ID : 4WF7
Title : Crystal structures of trehalose synthase from *Deinococcus radiodurans* reveal that a closed conformation is involved in the intramolecular isomerization catalysis
Authors : Wang, Y.L.; Chow, S.Y.; Lin, Y.T.; Hsieh, Y.C.; Lee, G.C.; Liaw, S.H.
Deposited on : 2014-09-13
Resolution : 2.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

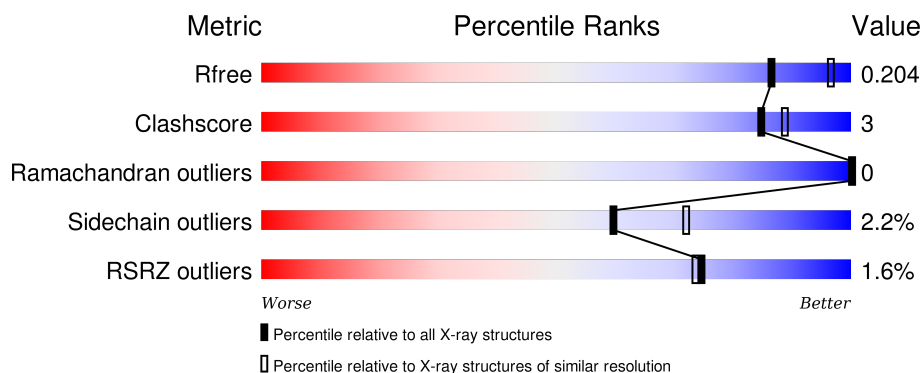
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	571	<div> <div>86%</div> <div>10%</div> <div>.</div> </div>
1	B	571	<div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	C	571	<div> <div>2%</div> <div>87%</div> <div>8%</div> <div>...</div> </div>
1	D	571	<div> <div>87%</div> <div>9%</div> <div>...</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	A	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18801 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
1	A	548	Total	C	N	O	S	0	0	0
			4401	2817	750	818	16			
1	B	548	Total	C	N	O	S	0	0	0
			4401	2817	750	818	16			
1	C	548	Total	C	N	O	S	0	0	0
			4401	2817	750	818	16			
1	D	548	Total	C	N	O	S	0	0	0
			4401	2817	750	818	16			

There are 96 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	253	ALA	ASN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	253	ALA	ASN	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	253	ALA	ASN	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	253	ALA	ASN	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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

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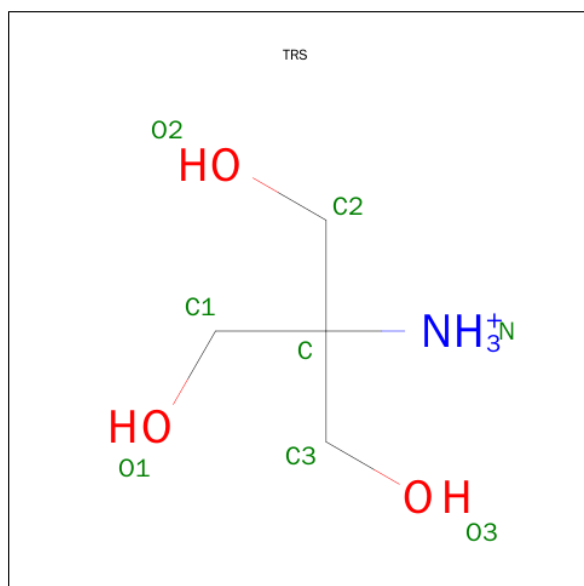
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		
4	C	1	Total	C	N	O	0	0
			8	4	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	N	O	0	0
			8	4	1	3		

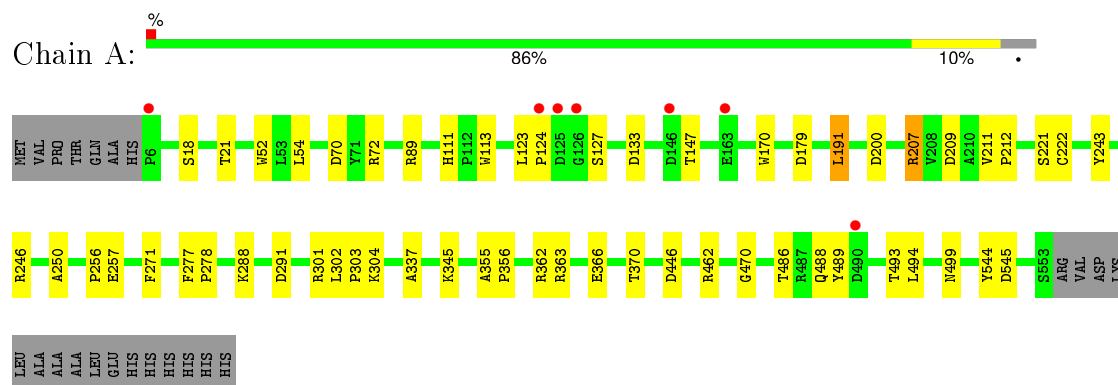
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	273	Total	O	0	0
			273	273		
5	B	333	Total	O	0	0
			333	333		
5	C	284	Total	O	0	0
			284	284		
5	D	259	Total	O	0	0
			259	259		

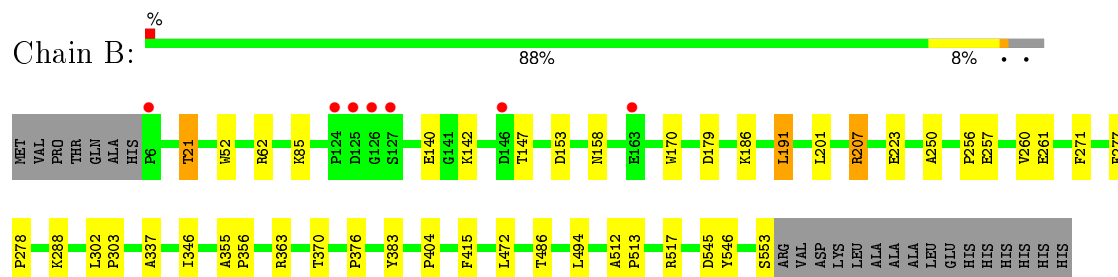
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

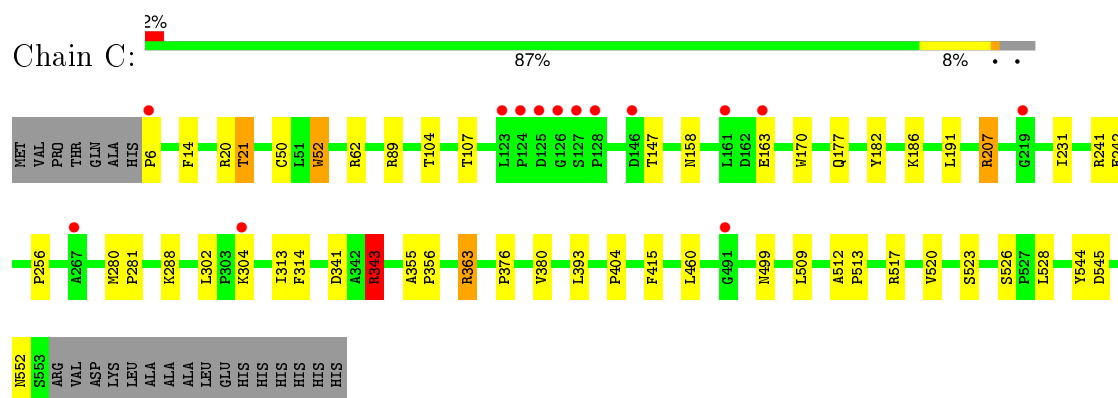
• Molecule 1: Trehalose synthase



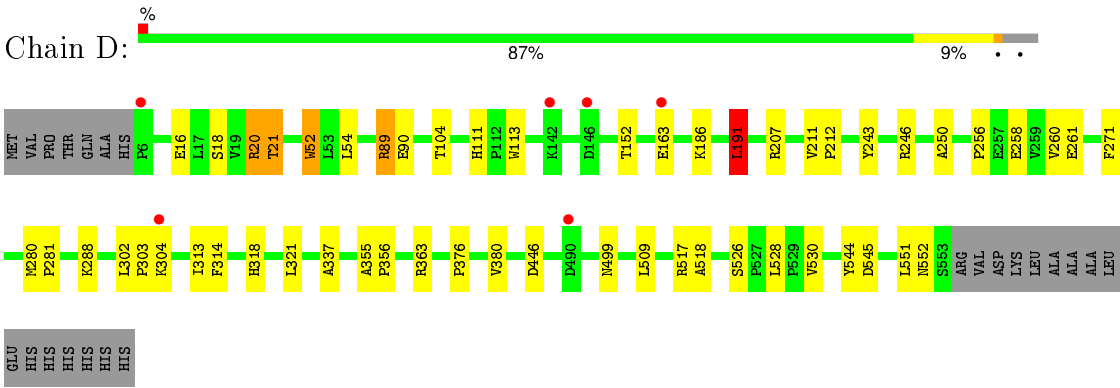
• Molecule 1: Trehalose synthase



• Molecule 1: Trehalose synthase



• Molecule 1: Trehalose synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.25Å 133.71Å 196.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.21 19.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.21) 99.3 (19.86-2.21)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.160 , 0.200 0.169 , 0.204	Depositor DCC
R_{free} test set	6336 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 126199 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18801	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.54	0/4534	0.74	10/6178 (0.2%)
1	B	0.55	0/4534	0.75	6/6178 (0.1%)
1	C	0.53	0/4534	0.74	9/6178 (0.1%)
1	D	0.54	0/4534	0.75	7/6178 (0.1%)
All	All	0.54	0/18136	0.75	32/24712 (0.1%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	B	363	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	C	20	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	363	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	363	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	D	20	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	20	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	207	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	363	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	D	363	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	C	207	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	B	207	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	363	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	191	LEU	CA-CB-CG	-6.29	100.82	115.30
1	C	363	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	72	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	89	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	207	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	462	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	D	191	LEU	CA-CB-CG	-5.72	102.15	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	C	343	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	70	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	62	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	446	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	363	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	191	LEU	CA-CB-CG	-5.30	103.10	115.30
1	C	89	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	446	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	191	LEU	CA-CB-CG	-5.09	103.60	115.30
1	A	89	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	291	ASP	CB-CG-OD1	5.02	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4401	0	4200	27	0
1	B	4401	0	4200	24	0
1	C	4401	0	4200	23	0
1	D	4401	0	4200	28	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
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
4	A	16	0	24	0	0
4	B	8	0	12	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
5	A	273	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	333	0	0	0	0
5	C	284	0	0	3	0
5	D	259	0	0	2	0
All	All	18801	0	16860	100	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 3.

All (100) 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:C:52:TRP:CZ2	1:C:207:ARG:HD3	2.13	0.84
1:A:52:TRP:CZ2	1:A:207:ARG:HD3	2.14	0.83
1:B:52:TRP:CZ2	1:B:207:ARG:HD3	2.15	0.81
1:B:517:ARG:HD3	1:B:553:SER:HA	1.71	0.72
1:A:52:TRP:CE2	1:A:207:ARG:HD3	2.25	0.72
1:A:147:THR:HG21	1:A:170:TRP:HH2	1.54	0.71
1:B:147:THR:HG21	1:B:170:TRP:HH2	1.58	0.67
1:B:260:VAL:HG21	1:B:303:PRO:HD2	1.75	0.67
1:D:517:ARG:HD2	1:D:552:ASN:O	1.95	0.66
1:D:52:TRP:CZ2	1:D:207:ARG:HD3	2.31	0.65
1:D:52:TRP:CE2	1:D:207:ARG:HD3	2.32	0.64
1:A:488:GLN:HG2	1:A:493:THR:HG23	1.82	0.61
1:D:260:VAL:HG21	1:D:303:PRO:HD2	1.82	0.61
1:D:20:ARG:NH2	5:D:811:HOH:O	2.35	0.60
1:B:52:TRP:CE2	1:B:207:ARG:HD3	2.37	0.59
1:C:341:ASP:OD2	1:C:343:ARG:HG3	2.03	0.58
1:C:52:TRP:CE2	1:C:207:ARG:HD3	2.40	0.57
1:C:62:ARG:NE	5:C:971:HOH:O	2.37	0.57
1:B:288:LYS:HG2	1:B:337:ALA:HB1	1.87	0.57
1:D:288:LYS:HG2	1:D:337:ALA:HB1	1.87	0.56
1:A:257:GLU:H	1:A:257:GLU:CD	2.10	0.55
1:D:313:ILE:HD11	1:D:376:PRO:O	2.07	0.54
1:A:288:LYS:HG2	1:A:337:ALA:HB1	1.90	0.53
1:B:355:ALA:HB3	1:B:356:PRO:HD3	1.90	0.53
1:A:366:GLU:O	1:A:370:THR:HG23	2.08	0.53
1:C:517:ARG:HD2	1:C:552:ASN:O	2.08	0.53
1:D:517:ARG:CD	1:D:552:ASN:O	2.58	0.52
1:A:18:SER:HB2	1:A:54:LEU:HD22	1.91	0.52
1:A:52:TRP:CZ2	1:A:207:ARG:CD	2.91	0.52
1:A:256:PRO:HB3	1:A:302:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:TYR:O	1:D:246:ARG:HG2	2.10	0.51
1:C:363:ARG:NH2	5:C:883:HOH:O	2.41	0.51
1:B:486:THR:HA	1:B:494:LEU:O	2.12	0.50
1:D:355:ALA:HB3	1:D:356:PRO:HD3	1.94	0.50
1:D:18:SER:HB2	1:D:54:LEU:HD22	1.94	0.50
1:C:280:MET:HB3	1:C:281:PRO:HD3	1.94	0.49
1:B:140:GLU:OE1	1:B:142:LYS:NZ	2.43	0.48
1:D:499:ASN:O	1:D:544:TYR:HA	2.14	0.48
1:B:376:PRO:HD3	1:B:472:LEU:HD13	1.95	0.48
1:C:313:ILE:HD11	1:C:376:PRO:O	2.13	0.48
1:B:147:THR:HG23	1:B:158:ASN:HD22	1.78	0.48
1:A:277:PHE:N	1:A:278:PRO:CD	2.77	0.47
1:A:486:THR:HA	1:A:494:LEU:O	2.14	0.47
1:A:211:VAL:N	1:A:212:PRO:CD	2.77	0.47
1:A:301:ARG:O	1:A:303:PRO:HD3	2.15	0.47
1:C:517:ARG:CD	1:C:552:ASN:O	2.62	0.47
1:B:21:THR:HG21	1:B:383:TYR:OH	2.14	0.47
1:C:147:THR:HG21	1:C:170:TRP:HH2	1.79	0.47
1:A:355:ALA:HB3	1:A:356:PRO:HD3	1.97	0.47
1:C:256:PRO:HB3	1:C:302:LEU:HD23	1.97	0.46
1:D:518:ALA:HB2	1:D:530:VAL:HG22	1.97	0.46
1:B:21:THR:CG2	1:B:383:TYR:OH	2.63	0.46
1:D:21:THR:HG22	5:D:784:HOH:O	2.15	0.46
1:B:404:PRO:HB3	1:B:415:PHE:CG	2.51	0.46
1:D:314:PHE:HB3	1:D:380:VAL:CG1	2.46	0.46
1:B:257:GLU:H	1:B:257:GLU:CD	2.19	0.46
1:D:211:VAL:N	1:D:212:PRO:CD	2.78	0.46
1:D:104:THR:HA	1:D:191:LEU:HD22	1.98	0.46
1:A:211:VAL:N	1:A:212:PRO:HD3	2.31	0.45
1:B:256:PRO:HB3	1:B:302:LEU:HD23	1.99	0.45
1:C:182:TYR:HB3	1:C:231:ILE:HD13	1.98	0.45
1:C:241:ARG:NH2	1:C:242:GLU:OE2	2.50	0.45
1:A:207:ARG:NH2	1:A:209:ASP:OD1	2.50	0.45
1:C:512:ALA:N	1:C:513:PRO:CD	2.79	0.45
1:B:370:THR:HG21	1:B:546:TYR:CD2	2.52	0.45
1:A:200:ASP:OD1	1:A:243:TYR:OH	2.27	0.45
1:C:499:ASN:O	1:C:544:TYR:HA	2.17	0.44
1:D:258:GLU:OE1	1:D:258:GLU:N	2.51	0.44
1:A:147:THR:HG21	1:A:170:TRP:CH2	2.43	0.43
1:C:355:ALA:HB3	1:C:356:PRO:HD3	2.00	0.43
1:B:85:LYS:HE2	1:B:201:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:LEU:HD23	1:D:321:LEU:C	2.39	0.43
1:D:280:MET:HB3	1:D:281:PRO:HD3	2.00	0.43
1:C:21:THR:HG22	5:C:829:HOH:O	2.18	0.43
1:B:277:PHE:N	1:B:278:PRO:CD	2.81	0.43
1:A:499:ASN:O	1:A:544:TYR:HA	2.19	0.43
1:C:14:PHE:HA	1:C:50:CYS:O	2.19	0.42
1:A:243:TYR:O	1:A:246:ARG:HG2	2.19	0.42
1:D:89:ARG:NH1	1:D:90:GLU:OE2	2.52	0.42
1:B:545:ASP:OD2	1:C:545:ASP:OD2	2.37	0.42
1:D:250:ALA:HB2	1:D:271:PHE:CG	2.55	0.42
1:D:111:HIS:CE1	1:D:113:TRP:CD2	3.07	0.42
1:D:16:GLU:OE2	1:D:318:HIS:ND1	2.46	0.42
1:C:147:THR:HG23	1:C:158:ASN:HD22	1.85	0.41
1:B:250:ALA:HB2	1:B:271:PHE:CG	2.55	0.41
1:A:470:GLY:HA2	1:A:489:TYR:HB2	2.02	0.41
1:D:551:LEU:HA	1:D:551:LEU:HD23	1.93	0.41
1:B:153:ASP:OD2	1:B:346:ILE:HA	2.20	0.41
1:A:221:SER:O	1:A:222:CYS:HB2	2.21	0.41
1:D:256:PRO:HB3	1:D:302:LEU:HD23	2.02	0.41
1:A:545:ASP:OD2	1:D:545:ASP:OD2	2.38	0.41
1:C:314:PHE:HB3	1:C:380:VAL:CG1	2.51	0.41
1:D:288:LYS:HG2	1:D:337:ALA:CB	2.51	0.41
1:C:404:PRO:HB3	1:C:415:PHE:CG	2.56	0.41
1:A:250:ALA:HB2	1:A:271:PHE:CG	2.56	0.41
1:B:260:VAL:HG11	1:B:303:PRO:HG2	2.02	0.40
1:A:111:HIS:CE1	1:A:113:TRP:CD2	3.09	0.40
1:A:123:LEU:HB3	1:A:124:PRO:HD2	2.03	0.40
1:B:512:ALA:N	1:B:513:PRO:CD	2.84	0.40
1:C:107:THR:O	1:C:177:GLN:HA	2.21	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	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%)	532 (97%)	14 (3%)	0	100	100
1	D	546/571 (96%)	531 (97%)	15 (3%)	0	100	100
All	All	2184/2284 (96%)	2127 (97%)	57 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	464/483 (96%)	456 (98%)	8 (2%)	68	80
1	B	464/483 (96%)	458 (99%)	6 (1%)	76	86
1	C	464/483 (96%)	448 (97%)	16 (3%)	44	54
1	D	464/483 (96%)	453 (98%)	11 (2%)	57	69
All	All	1856/1932 (96%)	1815 (98%)	41 (2%)	60	72

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	127	SER
1	A	133	ASP
1	A	179	ASP
1	A	191	LEU
1	A	304	LYS
1	A	345	LYS
1	A	362	ARG
1	B	21	THR
1	B	179	ASP
1	B	186	LYS
1	B	191	LEU
1	B	223	GLU

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Mol	Chain	Res	Type
1	B	261	GLU
1	C	6	PRO
1	C	21	THR
1	C	52	TRP
1	C	104	THR
1	C	163	GLU
1	C	186	LYS
1	C	288	LYS
1	C	304	LYS
1	C	343	ARG
1	C	393	LEU
1	C	460	LEU
1	C	509	LEU
1	C	520	VAL
1	C	523	SER
1	C	526	SER
1	C	528	LEU
1	D	21	THR
1	D	52	TRP
1	D	152	THR
1	D	163	GLU
1	D	186	LYS
1	D	191	LEU
1	D	261	GLU
1	D	304	LYS
1	D	509	LEU
1	D	526	SER
1	D	528	LEU

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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	A	602	-	7,7,7	0.84	0	9,9,9	0.89	0
4	TRS	A	603	-	7,7,7	0.63	0	9,9,9	1.40	1 (11%)
4	TRS	B	602	-	7,7,7	0.94	1 (14%)	9,9,9	1.17	1 (11%)
4	TRS	C	602	-	7,7,7	0.46	0	9,9,9	0.84	0
4	TRS	D	602	-	7,7,7	0.58	0	9,9,9	0.68	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	A	602	-	-	0/9/9/9	0/0/0/0
4	TRS	A	603	-	-	0/9/9/9	0/0/0/0
4	TRS	B	602	-	-	0/9/9/9	0/0/0/0
4	TRS	C	602	-	-	0/9/9/9	0/0/0/0
4	TRS	D	602	-	-	0/9/9/9	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	TRS	C-N	-2.22	1.47	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	602	TRS	C2-C-N	-2.21	104.07	108.09
4	A	603	TRS	C2-C-C1	2.51	116.22	110.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	548/571 (95%)	-0.46	7 (1%) 79 78	23, 31, 44, 70	0
1	B	548/571 (95%)	-0.50	7 (1%) 79 78	22, 30, 43, 66	0
1	C	548/571 (95%)	-0.36	14 (2%) 59 59	23, 33, 51, 79	0
1	D	548/571 (95%)	-0.39	6 (1%) 82 82	22, 32, 49, 73	0
All	All	2192/2284 (95%)	-0.43	34 (1%) 74 73	22, 31, 48, 79	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	146	ASP	5.0
1	A	146	ASP	4.9
1	B	6	PRO	4.5
1	C	124	PRO	3.9
1	A	124	PRO	3.9
1	B	146	ASP	3.7
1	D	146	ASP	3.4
1	D	163	GLU	3.3
1	C	125	ASP	3.3
1	C	6	PRO	3.2
1	B	163	GLU	3.1
1	A	163	GLU	3.1
1	D	304	LYS	3.1
1	D	490	ASP	3.0
1	B	124	PRO	3.0
1	C	163	GLU	3.0
1	A	6	PRO	2.8
1	C	126	GLY	2.8
1	A	125	ASP	2.8
1	C	127	SER	2.7
1	D	6	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	123	LEU	2.6
1	C	219	GLY	2.6
1	B	126	GLY	2.6
1	D	142	LYS	2.5
1	A	490	ASP	2.5
1	B	125	ASP	2.5
1	B	127	SER	2.3
1	C	267	ALA	2.2
1	C	304	LYS	2.2
1	C	161	LEU	2.2
1	C	491	GLY	2.1
1	C	128	PRO	2.1
1	A	126	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	TRS	A	603	8/8	0.86	0.23	8.60	49,53,55,55	0
4	TRS	B	602	8/8	0.97	0.09	0.02	25,28,30,34	0
4	TRS	A	602	8/8	0.95	0.10	-0.02	26,27,30,30	0
4	TRS	D	602	8/8	0.95	0.09	-0.05	31,34,35,35	0
4	TRS	C	602	8/8	0.97	0.09	-0.25	32,33,35,38	0
3	MG	D	601	1/1	0.99	0.07	-0.87	26,26,26,26	0
2	CA	D	600	1/1	1.00	0.09	-0.94	30,30,30,30	0
2	CA	A	600	1/1	0.99	0.08	-1.04	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	600	1/1	0.99	0.07	-1.74	26,26,26,26	0
2	CA	C	600	1/1	0.99	0.05	-1.96	35,35,35,35	0
3	MG	B	601	1/1	0.98	0.05	-2.28	21,21,21,21	0
3	MG	C	601	1/1	0.99	0.04	-2.37	23,23,23,23	0
3	MG	A	601	1/1	0.99	0.04	-2.59	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.