



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 02:11 AM BST

PDB ID : 5GTW  
Title : The N253R mutant structures of trehalose synthase from *Deinococcus radiodurans* display two different active-site conformations  
Authors : Chow, S.Y.; Wei, Y.J.; Liaw, S.H.  
Deposited on : 2016-08-23  
Resolution : 2.93 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1  
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) : 2.13.1

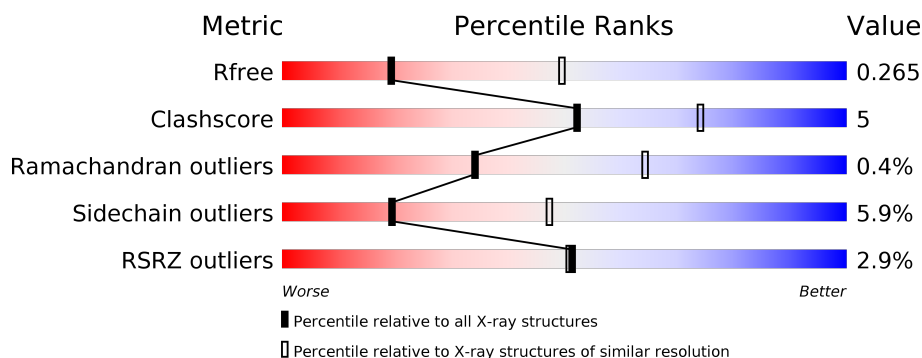
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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>2%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>••</div> </div> </div>
1	B	571	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>••</div> </div> </div>
1	C	571	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>••</div> </div> </div>
1	D	571	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17815 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
			4407	2820	753	818	16			
1	B	548	Total	C	N	O	S	0	0	0
			4407	2820	753	818	16			
1	C	548	Total	C	N	O	S	0	0	0
			4407	2820	753	818	16			
1	D	548	Total	C	N	O	S	0	0	0
			4407	2820	753	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	ARG	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	ARG	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	ARG	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	ARG	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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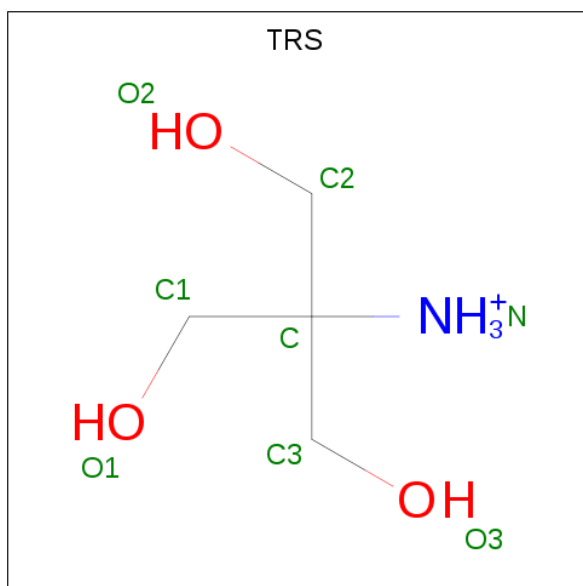
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		

- 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: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

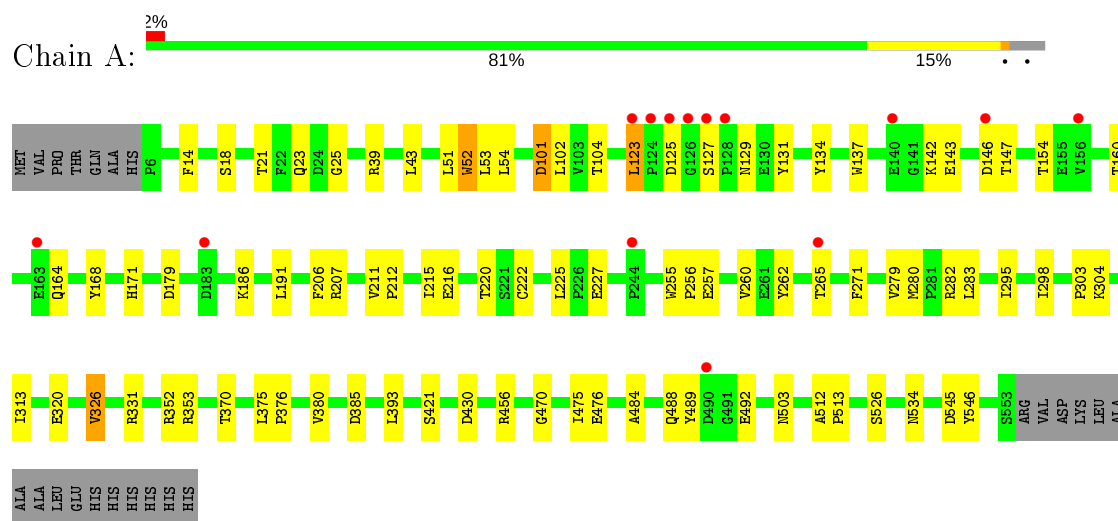
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total 43	O 43	0	0
5	B	33	Total 33	O 33	0	0
5	C	29	Total 29	O 29	0	0
5	D	50	Total 50	O 50	0	0

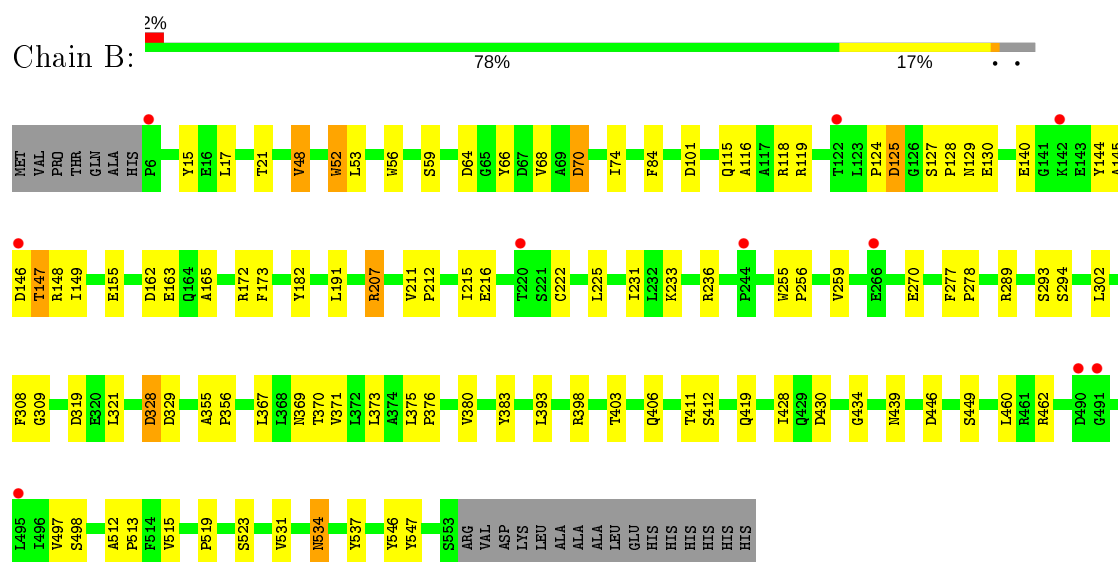
### 3 Residue-property plots

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.

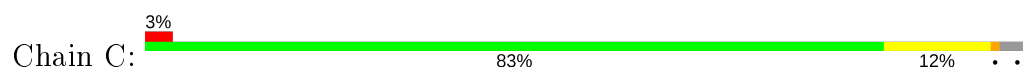
#### • Molecule 1: Trehalose synthase



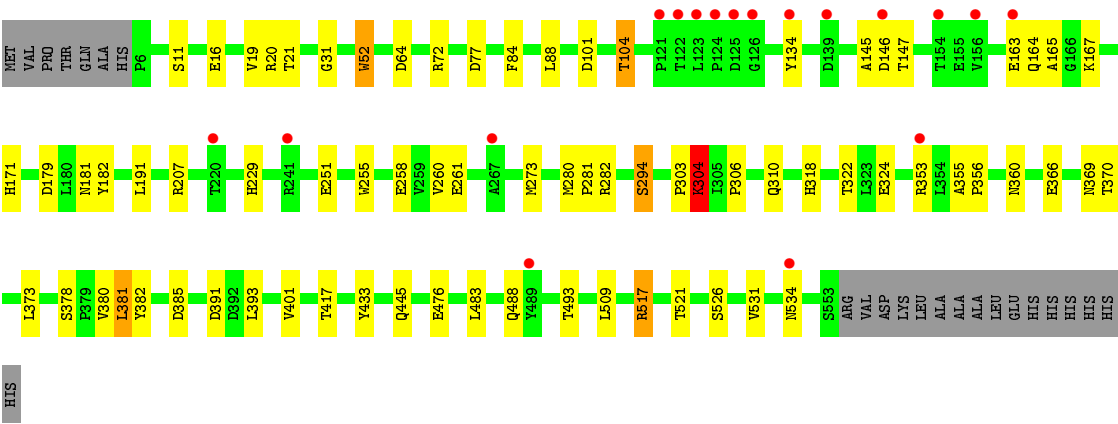
#### • Molecule 1: Trehalose synthase



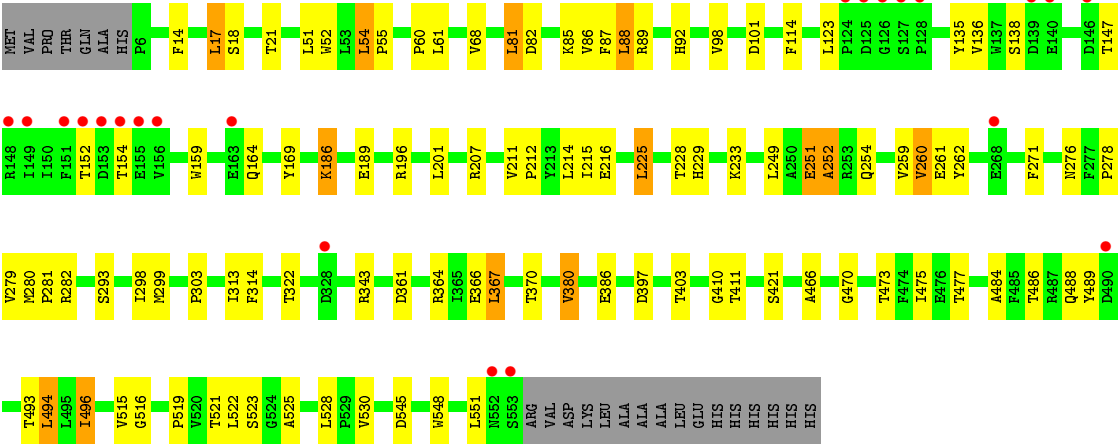
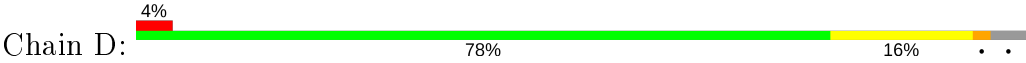
#### • Molecule 1: Trehalose synthase







● Molecule 1: Trehalose synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.38Å 134.06Å 197.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.93 19.93 – 2.93	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-2.93) 95.6 (19.93-2.93)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.81 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.182 , 0.267 0.186 , 0.265	Depositor DCC
$R_{free}$ test set	2696 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 65.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17815	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.67	0/4540	0.83	2/6185 (0.0%)
1	B	0.65	0/4540	0.79	0/6185
1	C	0.67	0/4540	0.80	1/6185 (0.0%)
1	D	0.67	0/4540	0.83	1/6185 (0.0%)
All	All	0.67	0/18160	0.81	4/24740 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	72	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	352	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	331	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	4407	0	4208	43	0
1	B	4407	0	4208	59	0
1	C	4407	0	4208	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4407	0	4208	49	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	8	0	12	0	0
4	B	8	0	12	2	0
4	C	8	0	12	1	0
5	A	43	0	0	2	0
5	B	33	0	0	1	0
5	C	29	0	0	0	0
5	D	50	0	0	0	0
All	All	17815	0	16868	189	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 5.

All (189) 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:A:160:THR:HG1	1:A:171:HIS:HE2	1.25	0.81
1:B:182:TYR:OH	1:B:191:LEU:HD13	1.81	0.78
1:C:366:GLU:O	1:C:370:THR:HG23	1.86	0.75
1:C:182:TYR:OH	1:C:191:LEU:HD22	1.88	0.74
1:B:236:ARG:NH1	1:B:270:GLU:O	2.24	0.69
1:D:215:ILE:H	1:D:228:THR:HG22	1.58	0.68
1:D:521:THR:O	1:D:525:ALA:HA	1.96	0.66
1:B:162:ASP:HB3	1:B:165:ALA:HB3	1.78	0.65
1:C:353:ARG:NH1	1:C:385:ASP:OD1	2.31	0.64
1:B:233:LYS:NZ	1:B:270:GLU:OE2	2.30	0.64
1:C:16:GLU:OE2	1:C:318:HIS:ND1	2.28	0.63
1:B:125:ASP:OD1	1:B:125:ASP:C	2.38	0.62
1:B:52:TRP:CZ2	1:B:207:ARG:HD3	2.35	0.61
1:B:328:ASP:N	1:B:328:ASP:OD1	2.33	0.60
1:D:260:VAL:HG11	1:D:303:PRO:HB2	1.83	0.60
1:B:255:TRP:O	1:B:259:VAL:HG23	2.02	0.59
1:D:279:VAL:HG11	1:D:299:MET:CE	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:TYR:O	1:D:271:PHE:HB2	2.04	0.57
1:D:229:HIS:O	1:D:233:LYS:HG3	2.04	0.57
1:B:148:ARG:O	1:B:172:ARG:NH2	2.38	0.56
1:C:260:VAL:HG21	1:C:303:PRO:HD2	1.88	0.56
1:A:104:THR:HG22	1:A:191:LEU:CD2	2.36	0.56
1:C:360:ASN:HB2	1:C:433:TYR:OH	2.06	0.56
1:D:466:ALA:HB3	1:D:494:LEU:HD22	1.87	0.56
1:B:125:ASP:OD1	1:B:125:ASP:O	2.25	0.55
1:B:127:SER:HB2	1:B:128:PRO:HD2	1.88	0.55
1:A:52:TRP:CZ2	1:A:207:ARG:HD3	2.41	0.54
1:B:145:ALA:O	1:B:146:ASP:HB2	2.06	0.54
1:C:171:HIS:O	1:C:171:HIS:ND1	2.41	0.54
1:B:256:PRO:HB3	1:B:302:LEU:HD23	1.90	0.53
1:A:260:VAL:HG21	1:A:303:PRO:HD2	1.89	0.53
1:C:381:LEU:HD23	1:C:381:LEU:N	2.23	0.53
1:A:220:THR:HB	5:A:736:HOH:O	2.07	0.53
1:C:534:ASN:N	1:C:534:ASN:OD1	2.42	0.53
1:B:277:PHE:N	1:B:278:PRO:CD	2.72	0.53
1:C:282:ARG:CG	1:C:294:SER:HB2	2.39	0.53
1:D:521:THR:CG2	1:D:523:SER:O	2.57	0.53
1:D:81:LEU:HD13	1:D:85:LYS:HE3	1.90	0.53
1:D:470:GLY:HA2	1:D:489:TYR:HB2	1.91	0.52
1:B:255:TRP:HE3	1:B:256:PRO:HD3	1.74	0.52
1:B:182:TYR:OH	1:B:191:LEU:CD1	2.56	0.52
1:B:173:PHE:CE1	4:B:603:TRS:H12	2.44	0.52
1:A:143:GLU:N	1:A:143:GLU:OE1	2.41	0.52
1:B:370:THR:HG21	1:B:546:TYR:CG	2.44	0.52
1:C:104:THR:HA	1:C:191:LEU:CD2	2.39	0.52
1:A:353:ARG:NH1	1:A:385:ASP:OD1	2.43	0.52
1:C:280:MET:HB3	1:C:281:PRO:HD3	1.91	0.51
1:B:70:ASP:OD1	1:B:70:ASP:C	2.49	0.51
1:B:66:TYR:HB3	4:B:603:TRS:O3	2.11	0.51
1:A:227:GLU:N	1:A:227:GLU:OE1	2.41	0.51
1:D:279:VAL:HG12	1:D:298:ILE:CG2	2.40	0.51
1:D:280:MET:HB3	1:D:281:PRO:HD3	1.92	0.51
1:C:229:HIS:CE1	1:C:261:GLU:HB3	2.46	0.50
1:A:370:THR:HG21	1:A:546:TYR:CG	2.46	0.50
1:A:25:GLY:HA3	1:C:417:THR:HG21	1.93	0.50
1:D:519:PRO:HA	1:D:551:LEU:HD23	1.93	0.50
1:A:222:CYS:HA	1:A:225:LEU:HD11	1.93	0.50
1:A:23:GLN:OE1	1:A:39:ARG:NH2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:PHE:CE1	1:C:88:LEU:HD22	2.46	0.50
1:B:534:ASN:N	1:B:534:ASN:OD1	2.45	0.50
1:C:521:THR:OG1	1:C:526:SER:N	2.42	0.50
1:B:222:CYS:HA	1:B:225:LEU:HD11	1.95	0.49
1:D:225:LEU:O	1:D:228:THR:OG1	2.26	0.49
1:B:446:ASP:HB3	1:B:449:SER:HB3	1.95	0.49
1:B:319:ASP:OD1	1:B:398:ARG:NH1	2.45	0.49
1:A:488:GLN:HA	1:A:492:GLU:O	2.13	0.49
1:C:134:TYR:O	1:C:181:ASN:HB3	2.13	0.49
1:B:17:LEU:HD12	1:B:17:LEU:C	2.33	0.49
1:B:215:ILE:HG22	1:B:216:GLU:N	2.28	0.49
1:B:512:ALA:O	1:B:515:VAL:HG23	2.12	0.49
1:D:52:TRP:CZ2	1:D:207:ARG:HD3	2.48	0.49
1:D:314:PHE:HB3	1:D:380:VAL:HG13	1.95	0.48
1:C:255:TRP:HB2	1:C:258:GLU:OE1	2.13	0.48
1:A:545:ASP:OD2	1:D:545:ASP:OD2	2.32	0.48
1:B:116:ALA:HA	1:B:119:ARG:HD2	1.95	0.48
1:D:136:VAL:O	1:D:169:TYR:HA	2.13	0.48
1:B:115:GLN:O	1:B:118:ARG:HG2	2.14	0.48
1:D:14:PHE:HB2	1:D:380:VAL:HB	1.95	0.48
1:A:125:ASP:OD1	1:A:127:SER:OG	2.32	0.48
1:B:215:ILE:HD11	1:B:231:ILE:HD11	1.96	0.48
1:A:475:ILE:HB	1:A:484:ALA:HB3	1.96	0.48
1:B:531:VAL:HG22	1:B:537:TYR:HD2	1.79	0.48
1:C:355:ALA:HB3	1:C:356:PRO:HD3	1.95	0.47
1:D:276:ASN:OD1	1:D:278:PRO:HD2	2.14	0.47
1:A:101:ASP:OD1	1:A:207:ARG:NE	2.45	0.47
1:D:60:PRO:O	1:D:61:LEU:HB2	2.14	0.47
1:D:54:LEU:HB3	1:D:55:PRO:HD2	1.95	0.47
1:C:517:ARG:O	1:C:531:VAL:HG23	2.14	0.47
1:D:279:VAL:HG11	1:D:299:MET:HE1	1.97	0.47
1:A:279:VAL:O	1:A:283:LEU:HG	2.15	0.47
1:B:56:TRP:CD1	1:B:74:ILE:HD13	2.50	0.47
1:D:366:GLU:O	1:D:367:LEU:C	2.51	0.47
1:C:488:GLN:CG	1:C:493:THR:HG23	2.45	0.47
1:D:366:GLU:O	1:D:370:THR:HG23	2.15	0.47
1:D:279:VAL:HG12	1:D:298:ILE:HG23	1.95	0.47
1:B:127:SER:HB2	1:B:128:PRO:CD	2.45	0.47
1:B:255:TRP:HB3	1:B:256:PRO:HD2	1.96	0.47
1:B:52:TRP:CE2	1:B:207:ARG:HD3	2.50	0.47
1:A:131:TYR:O	1:A:134:TYR:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ASN:O	1:C:373:LEU:HG	2.16	0.46
1:A:171:HIS:ND1	1:A:171:HIS:O	2.49	0.46
1:C:145:ALA:O	1:C:146:ASP:HB2	2.15	0.46
1:A:102:LEU:HB2	1:A:206:PHE:CD2	2.51	0.46
1:A:18:SER:HB2	1:A:54:LEU:HD22	1.97	0.46
1:B:53:LEU:HD12	1:B:53:LEU:N	2.31	0.46
1:A:456:ARG:NH2	5:A:702:HOH:O	2.49	0.45
1:B:531:VAL:HG22	1:B:537:TYR:CD2	2.51	0.45
1:C:488:GLN:HG3	1:C:493:THR:HG23	1.98	0.45
1:D:52:TRP:CD1	1:D:52:TRP:C	2.89	0.45
1:B:68:VAL:HG12	1:B:70:ASP:H	1.81	0.45
1:D:278:PRO:HB2	1:D:298:ILE:HG12	1.98	0.45
1:A:313:ILE:HD11	1:A:376:PRO:O	2.16	0.45
1:B:370:THR:HG21	1:B:546:TYR:CD2	2.52	0.45
1:D:17:LEU:CD2	1:D:17:LEU:C	2.85	0.45
1:A:160:THR:OG1	1:A:171:HIS:NE2	2.27	0.45
1:D:475:ILE:HG12	1:D:484:ALA:HB3	1.98	0.45
1:D:18:SER:HB2	1:D:54:LEU:HD23	1.98	0.45
1:C:165:ALA:O	1:C:167:LYS:HG3	2.17	0.45
1:C:260:VAL:HG21	1:C:303:PRO:HG2	1.98	0.44
1:C:273:MET:HG2	1:C:310:GLN:O	2.18	0.44
1:A:262:TYR:O	1:A:271:PHE:HB2	2.18	0.44
1:B:149:ILE:HG21	1:B:155:GLU:O	2.18	0.44
1:C:282:ARG:HG2	1:C:294:SER:HB2	2.00	0.44
1:D:17:LEU:O	1:D:17:LEU:HD22	2.18	0.44
1:A:375:LEU:HB3	1:A:376:PRO:HD2	1.99	0.44
1:A:52:TRP:C	1:A:52:TRP:CD1	2.90	0.44
1:B:144:TYR:O	1:B:147:THR:HB	2.17	0.44
1:B:411:THR:O	1:B:412:SER:C	2.56	0.44
1:C:20:ARG:HB2	1:C:20:ARG:NH1	2.33	0.43
1:D:278:PRO:O	1:D:282:ARG:HD2	2.17	0.43
1:C:171:HIS:O	1:C:171:HIS:CG	2.71	0.43
1:B:497:VAL:HB	1:B:547:TYR:HB2	2.01	0.43
1:C:380:VAL:C	1:C:381:LEU:HD23	2.38	0.43
1:C:251:GLU:OE2	4:C:603:TRS:O1	2.35	0.43
1:A:280:MET:HA	1:A:283:LEU:HD12	2.00	0.43
1:D:521:THR:HG22	1:D:523:SER:O	2.18	0.43
1:A:104:THR:HG22	1:A:191:LEU:HD23	2.01	0.43
1:C:322:THR:OG1	1:C:324:GLU:HG2	2.19	0.43
1:A:211:VAL:N	1:A:212:PRO:CD	2.81	0.43
1:A:534:ASN:OD1	1:A:534:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASN:O	1:B:130:GLU:C	2.57	0.43
1:C:19:VAL:O	1:C:31:GLY:HA3	2.19	0.43
1:B:428:ILE:HG22	1:B:434:GLY:HA2	2.00	0.42
1:D:251:GLU:O	1:D:252:ALA:HB2	2.19	0.42
1:B:383:TYR:O	1:B:383:TYR:CG	2.72	0.42
1:A:512:ALA:HB3	1:A:513:PRO:HD3	2.02	0.42
1:A:123:LEU:HD23	1:A:129:ASN:HB2	2.02	0.42
1:B:375:LEU:HB3	1:B:376:PRO:HD2	2.02	0.42
1:A:137:TRP:HA	1:A:168:TYR:O	2.20	0.42
1:C:104:THR:HG22	1:C:191:LEU:HD23	2.01	0.42
1:A:211:VAL:CG2	1:A:212:PRO:HD3	2.50	0.42
1:A:255:TRP:HB3	1:A:256:PRO:HD2	2.00	0.42
1:D:410:GLY:O	1:D:411:THR:C	2.59	0.42
1:D:88:LEU:HD22	1:D:92:HIS:CE1	2.54	0.42
1:B:406:GLN:O	1:B:439:ASN:HA	2.20	0.41
1:B:211:VAL:N	1:B:212:PRO:CD	2.84	0.41
1:B:255:TRP:HB3	1:B:256:PRO:CD	2.51	0.41
1:B:308:PHE:CD1	1:B:309:GLY:N	2.87	0.41
1:B:512:ALA:N	1:B:513:PRO:CD	2.83	0.41
1:B:84:PHE:C	1:B:84:PHE:CD1	2.93	0.41
1:D:211:VAL:CG2	1:D:212:PRO:HD3	2.50	0.41
1:C:303:PRO:O	1:C:304:LYS:C	2.59	0.41
1:D:486:THR:HA	1:D:494:LEU:O	2.20	0.41
1:C:273:MET:HA	1:C:310:GLN:O	2.20	0.41
1:A:215:ILE:O	1:A:225:LEU:HD12	2.20	0.41
1:B:289:ARG:CG	5:B:722:HOH:O	2.68	0.41
1:D:488:GLN:HG3	1:D:493:THR:HG23	2.03	0.41
1:D:522:LEU:HD22	1:D:548:TRP:HB3	2.02	0.41
1:A:295:ILE:O	1:A:298:ILE:HG22	2.21	0.41
1:B:293:SER:O	1:B:294:SER:C	2.59	0.41
1:D:138:SER:HB2	1:D:159:TRP:CH2	2.55	0.41
1:B:355:ALA:HB3	1:B:356:PRO:HD3	2.02	0.41
1:B:367:LEU:O	1:B:371:VAL:HG23	2.20	0.41
1:D:361:ASP:OD2	1:D:364:ARG:HG3	2.21	0.41
1:D:515:VAL:HG12	1:D:516:GLY:N	2.35	0.41
1:B:369:ASN:O	1:B:373:LEU:HG	2.21	0.41
1:C:52:TRP:CZ2	1:C:207:ARG:HD3	2.56	0.41
1:D:259:VAL:O	1:D:261:GLU:N	2.54	0.41
1:A:14:PHE:CD1	1:A:14:PHE:N	2.89	0.41
1:D:186:LYS:O	1:D:189:GLU:HB2	2.21	0.41
1:A:282:ARG:NH2	1:A:326:VAL:HG12	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:TYR:HB2	1:B:48:VAL:HG21	2.02	0.40
1:D:496:ILE:O	1:D:496:ILE:HG13	2.21	0.40
1:A:470:GLY:HA2	1:A:489:TYR:HB2	2.02	0.40
1:D:211:VAL:HG22	1:D:212:PRO:HD3	2.03	0.40
1:C:382:TYR:OH	1:C:401:VAL:O	2.28	0.40
1:A:43:LEU:HD13	1:A:51:LEU:CD2	2.52	0.40
1:C:273:MET:HE1	1:C:378:SER:HB2	2.04	0.40
1:D:114:PHE:HB2	1:D:135:TYR:CZ	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	546/571 (96%)	514 (94%)	32 (6%)	0	100	100
1	B	546/571 (96%)	509 (93%)	34 (6%)	3 (0%)	29	60
1	C	546/571 (96%)	498 (91%)	45 (8%)	3 (0%)	29	60
1	D	546/571 (96%)	510 (93%)	33 (6%)	3 (0%)	29	60
All	All	2184/2284 (96%)	2031 (93%)	144 (7%)	9 (0%)	34	64

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	304	LYS
1	D	214	LEU
1	D	252	ALA
1	B	70	ASP
1	C	77	ASP
1	B	534	ASN
1	B	124	PRO

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Mol	Chain	Res	Type
1	C	306	PRO
1	D	260	VAL

### 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	465/484 (96%)	440 (95%)	25 (5%)	22	51
1	B	465/484 (96%)	441 (95%)	24 (5%)	23	53
1	C	465/484 (96%)	445 (96%)	20 (4%)	29	60
1	D	465/484 (96%)	424 (91%)	41 (9%)	10	28
All	All	1860/1936 (96%)	1750 (94%)	110 (6%)	19	47

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	THR
1	A	52	TRP
1	A	53	LEU
1	A	101	ASP
1	A	123	LEU
1	A	142	LYS
1	A	146	ASP
1	A	147	THR
1	A	154	THR
1	A	164	GLN
1	A	179	ASP
1	A	186	LYS
1	A	216	GLU
1	A	257	GLU
1	A	265	THR
1	A	304	LYS
1	A	320	GLU
1	A	326	VAL
1	A	380	VAL

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Mol	Chain	Res	Type
1	A	393	LEU
1	A	421	SER
1	A	430	ASP
1	A	476	GLU
1	A	503	ASN
1	A	526	SER
1	B	21	THR
1	B	48	VAL
1	B	52	TRP
1	B	59	SER
1	B	64	ASP
1	B	101	ASP
1	B	125	ASP
1	B	140	GLU
1	B	147	THR
1	B	163	GLU
1	B	207	ARG
1	B	321	LEU
1	B	328	ASP
1	B	329	ASP
1	B	380	VAL
1	B	393	LEU
1	B	403	THR
1	B	419	GLN
1	B	430	ASP
1	B	460	LEU
1	B	462	ARG
1	B	498	SER
1	B	519	PRO
1	B	523	SER
1	C	11	SER
1	C	21	THR
1	C	52	TRP
1	C	64	ASP
1	C	101	ASP
1	C	104	THR
1	C	147	THR
1	C	163	GLU
1	C	164	GLN
1	C	179	ASP
1	C	294	SER
1	C	304	LYS

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Mol	Chain	Res	Type
1	C	381	LEU
1	C	391	ASP
1	C	393	LEU
1	C	445	GLN
1	C	476	GLU
1	C	483	LEU
1	C	509	LEU
1	C	517	ARG
1	D	17	LEU
1	D	21	THR
1	D	51	LEU
1	D	54	LEU
1	D	68	VAL
1	D	81	LEU
1	D	82	ASP
1	D	86	VAL
1	D	87	PHE
1	D	88	LEU
1	D	98	VAL
1	D	101	ASP
1	D	123	LEU
1	D	147	THR
1	D	152	THR
1	D	154	THR
1	D	164	GLN
1	D	186	LYS
1	D	196	ARG
1	D	201	LEU
1	D	216	GLU
1	D	225	LEU
1	D	249	LEU
1	D	251	GLU
1	D	254	GLN
1	D	293	SER
1	D	313	ILE
1	D	322	THR
1	D	343	ARG
1	D	367	LEU
1	D	380	VAL
1	D	386	GLU
1	D	397	ASP
1	D	403	THR

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Mol	Chain	Res	Type
1	D	421	SER
1	D	473	THR
1	D	477	THR
1	D	494	LEU
1	D	496	ILE
1	D	528	LEU
1	D	530	VAL

Some 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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	B	603	-	7,7,7	0.34	0	9,9,9	0.74	0
4	TRS	C	603	-	7,7,7	0.34	0	9,9,9	1.00	1 (11%)
4	TRS	A	603	-	7,7,7	0.55	0	9,9,9	0.95	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	B	603	-	-	3/9/9/9	-
4	TRS	C	603	-	-	6/9/9/9	-
4	TRS	A	603	-	-	6/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	TRS	C3-C-N	2.26	114.72	107.98

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	TRS	C2-C-C3-O3
4	C	603	TRS	C2-C-C1-O1
4	C	603	TRS	C3-C-C1-O1
4	C	603	TRS	N-C-C1-O1
4	C	603	TRS	C1-C-C3-O3
4	C	603	TRS	C2-C-C3-O3
4	C	603	TRS	N-C-C3-O3
4	A	603	TRS	C3-C-C1-O1
4	A	603	TRS	C3-C-C2-O2
4	A	603	TRS	N-C-C2-O2
4	B	603	TRS	C1-C-C3-O3
4	A	603	TRS	C2-C-C1-O1
4	A	603	TRS	N-C-C1-O1
4	A	603	TRS	C1-C-C2-O2
4	B	603	TRS	N-C-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	TRS	2	0
4	C	603	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	548/571 (95%)	-0.29	14 (2%) 56 56	21, 51, 80, 115	3 (0%)
1	B	548/571 (95%)	-0.27	10 (1%) 68 69	24, 52, 80, 98	3 (0%)
1	C	548/571 (95%)	-0.19	18 (3%) 46 45	23, 55, 82, 126	3 (0%)
1	D	548/571 (95%)	-0.18	22 (4%) 38 37	25, 52, 90, 130	3 (0%)
All	All	2192/2284 (95%)	-0.23	64 (2%) 51 51	21, 53, 82, 130	12 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	146	ASP	6.9
1	C	146	ASP	4.0
1	D	153	ASP	4.0
1	D	152	THR	3.8
1	D	156	VAL	3.8
1	B	146	ASP	3.7
1	C	124	PRO	3.5
1	C	125	ASP	3.4
1	A	126	GLY	3.4
1	C	163	GLU	3.3
1	C	126	GLY	3.3
1	D	127	SER	3.2
1	D	139	ASP	3.2
1	A	127	SER	3.2
1	D	124	PRO	3.1
1	D	154	THR	3.1
1	C	123	LEU	3.1
1	B	142	LYS	3.1
1	C	122	THR	3.0
1	A	123	LEU	3.0
1	A	146	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	156	VAL	2.9
1	A	125	ASP	2.9
1	C	121	PRO	2.8
1	D	328	ASP	2.8
1	D	490	ASP	2.8
1	D	163	GLU	2.8
1	A	124	PRO	2.8
1	D	125	ASP	2.7
1	D	155	GLU	2.7
1	A	244	PRO	2.7
1	A	183	ASP	2.6
1	B	495	LEU	2.5
1	C	220	THR	2.5
1	A	490	ASP	2.5
1	B	6	PRO	2.5
1	C	267	ALA	2.5
1	A	156	VAL	2.5
1	D	140	GLU	2.5
1	D	126	GLY	2.5
1	C	139	ASP	2.5
1	C	534	ASN	2.4
1	B	220	THR	2.4
1	D	151	PHE	2.4
1	D	268	GLU	2.4
1	B	490	ASP	2.3
1	D	552	ASN	2.3
1	A	140	GLU	2.3
1	D	149	ILE	2.3
1	B	244	PRO	2.2
1	C	134	TYR	2.2
1	B	266	GLU	2.2
1	D	148	ARG	2.2
1	C	154	THR	2.2
1	B	122	THR	2.2
1	D	553	SER	2.1
1	B	491	GLY	2.1
1	C	489	TYR	2.1
1	A	265	THR	2.1
1	C	353	ARG	2.1
1	C	241	ARG	2.1
1	A	163	GLU	2.0
1	D	128	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	128	PRO	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	TRS	A	603	8/8	0.86	0.28	63,75,83,83	0
4	TRS	B	603	8/8	0.92	0.19	64,79,83,88	0
4	TRS	C	603	8/8	0.94	0.21	57,62,72,80	0
3	MG	B	602	1/1	0.95	0.47	63,63,63,63	0
2	CA	B	601	1/1	0.95	0.21	78,78,78,78	0
3	MG	C	602	1/1	0.96	0.07	40,40,40,40	0
3	MG	D	601	1/1	0.97	0.09	35,35,35,35	0
3	MG	A	602	1/1	0.97	0.06	29,29,29,29	0
2	CA	C	601	1/1	0.98	0.10	59,59,59,59	0
2	CA	A	601	1/1	0.99	0.19	57,57,57,57	0
2	CA	D	600	1/1	0.99	0.18	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.