



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:23 PM GMT

PDB ID : 1G3L  
Title : THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND  
REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSF  
ERASE(RMLA). TDP-L-RHAMNOSE COMPLEX.  
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Deposited on : 2000-10-24  
Resolution : 2.70 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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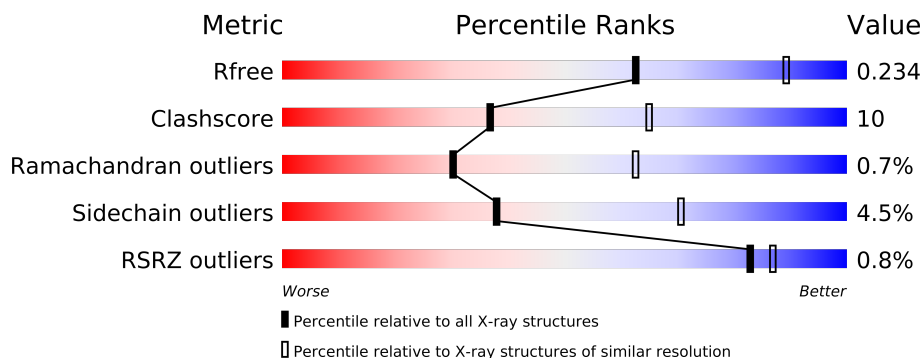
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	293	
1	B	293	
1	C	293	
1	D	293	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	700	-	X
2	SO4	C	703	-	X
2	SO4	D	704	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9453 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	B	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	C	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	D	293	Total	C	N	O	S	0	0	0
			2293	1467	386	435	5			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



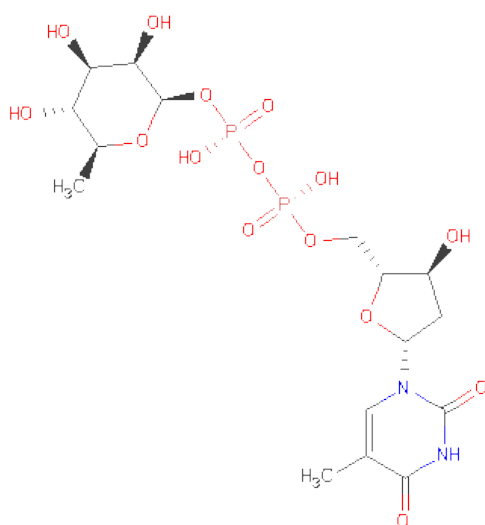
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is 2'-DEOXY-THYMIDINE-BETA-L-RHAMNOSE (three-letter code: TRH) (formula: C<sub>16</sub>H<sub>26</sub>N<sub>2</sub>O<sub>15</sub>P<sub>2</sub>).



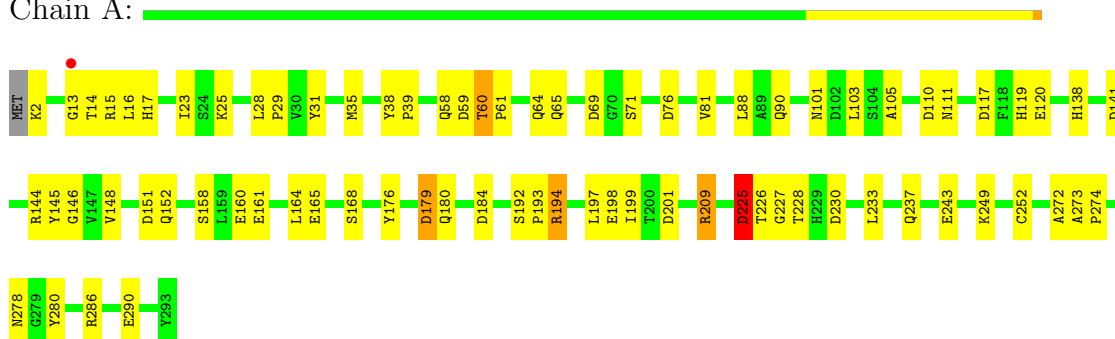
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	A	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	B	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	B	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	C	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	C	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	D	1	Total	C	N	O	P	0	0
			35	16	2	15	2		
3	D	1	Total	C	N	O	P	0	0
			35	16	2	15	2		

### 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 ( $RSRZ > 2$ ). 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.

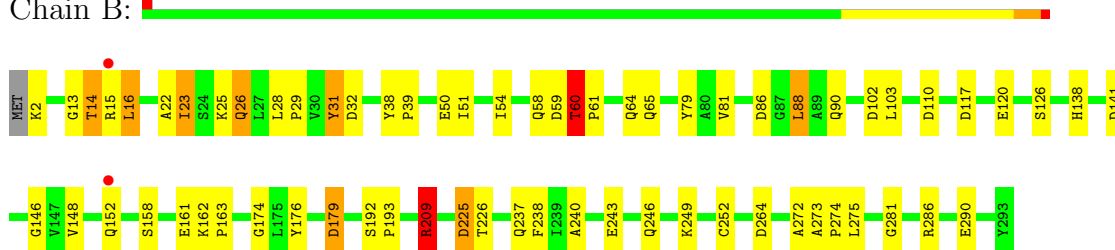
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

Chain A:



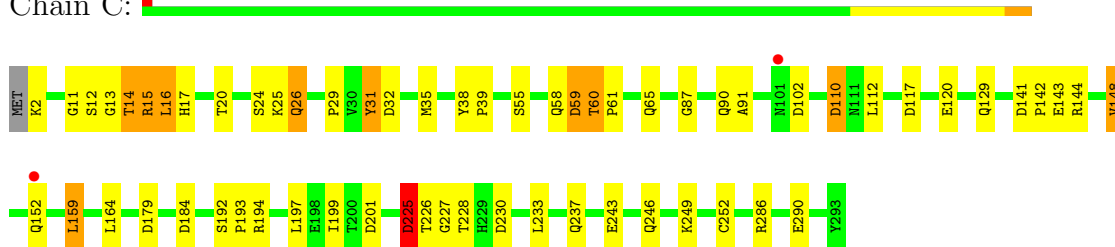
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

Chain B:



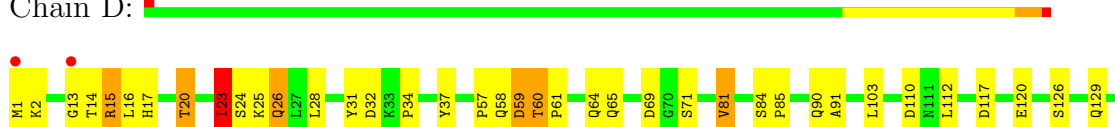
#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

Chain C:



#### • Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLTRANSFERASE

Chain D:



H138	D141	P142	E143	V147	V148	E149	F150	L164	S168	S192	P193	R194	L197	E198	I199	T200	D201	S213	D225	T226	G227	T228	H229	L233	Q237	F238	E243	Q246	C252	D264	A273	P274	Y293
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.09Å 138.56Å 139.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 49.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.8 (100.00-2.70) 93.8 (49.82-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.204 , 0.230 0.213 , 0.234	Depositor DCC
$R_{free}$ test set	1815 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.0	Xtriage
Anisotropy	0.449	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , -7.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 36278 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.00 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.9405e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRH, SO4

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	0.91	0/2335	1.01	10/3168 (0.3%)
1	B	0.89	1/2335 (0.0%)	1.02	12/3168 (0.4%)
1	C	0.86	0/2335	1.03	13/3168 (0.4%)
1	D	0.89	1/2343 (0.0%)	1.01	10/3178 (0.3%)
All	All	0.89	2/9348 (0.0%)	1.02	45/12682 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	ARG	CB-CG	-5.11	1.38	1.52
1	D	23	ILE	CA-CB	-5.03	1.43	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ASP	CB-CG-OD2	8.76	126.18	118.30
1	C	59	ASP	CB-CG-OD2	7.28	124.85	118.30
1	A	184	ASP	CB-CG-OD2	7.07	124.67	118.30
1	B	59	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	225	ASP	CB-CG-OD2	6.80	124.42	118.30
1	C	152	GLN	CA-CB-CG	-6.77	98.51	113.40
1	C	110	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	ASP	CB-CG-OD2	6.62	124.26	118.30
1	D	59	ASP	CB-CG-OD2	6.51	124.16	118.30
1	D	117	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	209	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	209	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	201	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	152	GLN	CA-CB-CG	-6.04	100.12	113.40
1	A	76	ASP	CB-CG-OD2	5.98	123.69	118.30
1	D	110	ASP	CB-CG-OD2	5.95	123.65	118.30
1	D	201	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	179	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	102	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	141	ASP	CB-CG-OD2	5.78	123.50	118.30
1	D	15	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	110	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	194	ARG	CB-CA-C	-5.70	99.00	110.40
1	B	141	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	201	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	117	ASP	CB-CG-OD2	5.57	123.32	118.30
1	C	117	ASP	CB-CG-OD2	5.57	123.32	118.30
1	C	230	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	194	ARG	CB-CA-C	-5.49	99.43	110.40
1	D	225	ASP	CB-CA-C	5.48	121.36	110.40
1	C	194	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	117	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	16	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	60	THR	OG1-CB-CG2	-5.34	97.72	110.00
1	B	179	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	194	ARG	CB-CA-C	-5.27	99.86	110.40
1	A	230	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	225	ASP	CB-CA-C	5.24	120.87	110.40
1	B	86	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	209	ARG	CB-CA-C	-5.13	100.14	110.40
1	D	141	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	59	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	264	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	159	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	D	15	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	HIS	Sidechain
1	A	17	HIS	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2285	0	2272	50	0
1	B	2285	0	2272	49	0
1	C	2285	0	2272	55	0
1	D	2293	0	2284	56	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	1	0
3	A	70	0	48	1	0
3	B	70	0	48	0	0
3	C	70	0	48	3	0
3	D	70	0	48	1	0
All	All	9453	0	9292	192	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (192) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:GLU:N	1:B:120:GLU:OE1	2.07	0.88
1:C:58:GLN:HE22	1:D:65:GLN:HE22	1.23	0.84
1:C:141:ASP:OD2	1:C:144:ARG:HD3	1.78	0.83
1:D:120:GLU:N	1:D:120:GLU:OE1	2.17	0.78
1:C:58:GLN:NE2	1:D:65:GLN:HE22	1.81	0.78
1:B:273:ALA:HB3	1:B:274:PRO:HD3	1.66	0.78
1:C:26:GLN:NE2	1:C:26:GLN:H	1.82	0.77
1:A:237:GLN:OE1	1:B:237:GLN:NE2	2.17	0.76
1:D:26:GLN:H	1:D:26:GLN:HE21	1.32	0.75
1:A:13:GLY:O	1:A:16:LEU:N	2.21	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:69:ASP:OD1	1:D:71:SER:OG	2.06	0.73
1:A:120:GLU:OE1	1:A:120:GLU:N	2.21	0.73
1:C:120:GLU:N	1:C:120:GLU:OE1	2.21	0.72
1:C:60:THR:HB	1:C:61:PRO:HD3	1.73	0.71
1:D:13:GLY:O	1:D:16:LEU:N	2.23	0.70
1:C:141:ASP:HB2	1:C:143:GLU:OE2	1.91	0.70
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.73	0.70
1:A:25:LYS:NZ	1:A:226:THR:O	2.24	0.69
1:B:88:LEU:N	1:B:88:LEU:HD23	2.08	0.68
1:C:26:GLN:HE21	1:C:26:GLN:H	1.41	0.67
1:B:60:THR:HG22	1:B:61:PRO:N	2.10	0.67
1:A:58:GLN:HE22	1:B:65:GLN:HE22	1.41	0.67
1:A:65:GLN:HE22	1:B:58:GLN:HE22	1.40	0.67
1:A:25:LYS:HE3	1:A:226:THR:O	1.96	0.66
1:C:2:LYS:HG3	1:C:2:LYS:O	1.96	0.65
1:D:26:GLN:H	1:D:26:GLN:NE2	1.94	0.65
1:B:13:GLY:O	1:B:14:THR:C	2.35	0.63
1:D:1:MET:N	1:D:129:GLN:HE21	1.97	0.63
1:D:25:LYS:HE3	1:D:226:THR:O	1.99	0.63
1:A:28:LEU:HD22	1:B:29:PRO:HD3	1.81	0.62
1:B:209:ARG:HH11	1:B:209:ARG:HG2	1.63	0.62
1:C:58:GLN:HE22	1:D:65:GLN:NE2	1.96	0.61
1:A:225:ASP:C	1:A:225:ASP:OD1	2.39	0.60
1:A:144:ARG:NH2	1:A:145:TYR:OH	2.34	0.60
1:A:60:THR:HB	1:A:61:PRO:HD3	1.84	0.60
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.82	0.60
1:D:1:MET:CE	1:D:103:LEU:HD21	2.31	0.59
1:A:25:LYS:CE	1:A:226:THR:O	2.51	0.59
1:D:25:LYS:NZ	1:D:226:THR:O	2.36	0.59
1:C:11:GLY:HA3	3:C:504:TRH:H2'1	1.85	0.58
1:B:64:GLN:HG2	1:B:79:TYR:CE1	2.39	0.58
1:D:25:LYS:CE	1:D:226:THR:O	2.51	0.58
1:A:23:ILE:HG12	1:B:23:ILE:HG12	1.86	0.58
1:A:13:GLY:O	1:A:14:THR:C	2.43	0.57
1:A:14:THR:O	1:A:15:ARG:C	2.40	0.57
1:C:60:THR:HG22	1:C:61:PRO:N	2.18	0.57
1:C:142:PRO:HD2	1:C:143:GLU:OE1	2.04	0.57
1:A:60:THR:HG22	1:A:61:PRO:N	2.15	0.56
1:B:192:SER:HB2	1:B:193:PRO:CD	2.36	0.56
1:C:60:THR:CB	1:C:61:PRO:HD3	2.35	0.56
1:A:101:ASN:O	1:A:180:GLN:NE2	2.31	0.55
1:B:16:LEU:HD12	1:B:25:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:23:ILE:HD12	1:D:28:LEU:HD21	1.87	0.55
1:A:69:ASP:OD1	1:A:71:SER:OG	2.15	0.55
1:D:13:GLY:O	1:D:14:THR:C	2.44	0.55
1:B:23:ILE:H	1:B:23:ILE:HD12	1.72	0.55
1:D:1:MET:HE3	1:D:103:LEU:HD21	1.88	0.54
1:C:25:LYS:HE2	1:C:110:ASP:HB2	1.89	0.54
1:C:129:GLN:N	2:C:703:SO4:O4	2.39	0.54
1:A:110:ASP:OD2	3:A:500:TRH:O3'	2.16	0.53
1:C:179:ASP:OD1	1:C:179:ASP:C	2.46	0.53
1:C:29:PRO:HD3	1:D:28:LEU:HD22	1.92	0.53
1:D:60:THR:HG23	1:D:64:GLN:OE1	2.08	0.52
1:C:24:SER:HB3	1:C:26:GLN:HE22	1.73	0.52
1:D:60:THR:HG22	1:D:61:PRO:N	2.23	0.52
1:B:179:ASP:OD1	1:B:179:ASP:C	2.48	0.52
1:D:32:ASP:OD2	1:D:243:GLU:OE1	2.28	0.52
1:B:243:GLU:HG2	1:B:249:LYS:HA	1.92	0.52
1:C:225:ASP:OD1	1:C:225:ASP:C	2.48	0.52
1:A:65:GLN:NE2	1:B:58:GLN:HE22	2.06	0.52
1:D:1:MET:HB2	1:D:103:LEU:HD11	1.92	0.52
1:D:129:GLN:N	2:D:704:SO4:O1	2.23	0.52
1:C:14:THR:O	1:C:15:ARG:C	2.47	0.52
1:C:14:THR:O	1:C:15:ARG:O	2.28	0.52
1:C:31:TYR:CE1	1:D:229:HIS:HB3	2.46	0.51
1:C:112:LEU:C	1:C:112:LEU:HD23	2.30	0.51
1:A:286:ARG:NH1	1:A:290:GLU:OE1	2.40	0.51
1:B:14:THR:O	1:B:15:ARG:C	2.49	0.51
1:C:38:TYR:HB2	1:C:39:PRO:CD	2.40	0.51
1:B:138:HIS:ND1	1:D:246:GLN:O	2.43	0.51
1:B:225:ASP:OD1	1:B:225:ASP:C	2.49	0.51
1:A:2:LYS:HG3	1:A:2:LYS:O	2.09	0.51
1:D:273:ALA:N	1:D:274:PRO:CD	2.74	0.51
1:B:103:LEU:HD23	1:B:179:ASP:HA	1.93	0.51
1:C:25:LYS:HE2	1:C:110:ASP:CB	2.41	0.50
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.93	0.50
1:A:278:ASN:OD1	1:A:280:TYR:N	2.45	0.50
1:D:141:ASP:HB3	1:D:143:GLU:OE2	2.11	0.50
1:D:24:SER:OG	1:D:59:ASP:OD2	2.17	0.49
1:A:38:TYR:HB2	1:A:39:PRO:CD	2.43	0.49
1:A:194:ARG:NH2	1:A:198:GLU:OE1	2.41	0.49
1:A:273:ALA:N	1:A:274:PRO:CD	2.76	0.49
1:D:1:MET:H3	1:D:129:GLN:HE21	1.61	0.49
1:C:13:GLY:O	1:C:14:THR:C	2.49	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:PRO:HD3	1:B:28:LEU:HD22	1.96	0.48
1:D:60:THR:N	1:D:61:PRO:HD2	2.29	0.48
1:C:60:THR:CB	1:C:61:PRO:CD	2.91	0.48
1:A:272:ALA:O	1:A:273:ALA:C	2.52	0.48
1:C:227:GLY:C	1:C:228:THR:CG2	2.81	0.48
1:D:112:LEU:HD23	1:D:112:LEU:C	2.34	0.48
1:B:2:LYS:HG3	1:B:2:LYS:O	2.12	0.47
1:B:162:LYS:N	1:B:163:PRO:CD	2.77	0.47
1:A:227:GLY:O	1:A:228:THR:HG22	2.14	0.47
1:B:146:GLY:HA2	1:B:161:GLU:HA	1.96	0.47
1:A:164:LEU:C	1:A:165:GLU:HG2	2.34	0.47
1:D:60:THR:N	1:D:61:PRO:CD	2.77	0.47
1:B:246:GLN:O	1:D:138:HIS:ND1	2.41	0.47
1:D:164:LEU:HA	1:D:164:LEU:HD23	1.83	0.47
1:B:50:GLU:C	1:B:51:ILE:HG13	2.35	0.47
1:C:60:THR:O	1:C:61:PRO:C	2.52	0.46
1:B:23:ILE:HD12	1:B:23:ILE:N	2.31	0.46
1:A:105:ALA:HA	1:A:176:TYR:O	2.15	0.46
1:A:35:MET:SD	1:A:110:ASP:HA	2.55	0.46
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.48	0.46
1:A:25:LYS:HZ2	1:A:226:THR:C	2.19	0.46
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.98	0.46
1:A:103:LEU:HD23	1:A:179:ASP:HA	1.98	0.46
1:B:209:ARG:HG2	1:B:209:ARG:NH1	2.30	0.45
1:A:60:THR:CB	1:A:61:PRO:HD3	2.45	0.45
1:C:233:LEU:HD12	1:C:233:LEU:HA	1.57	0.45
1:D:90:GLN:O	1:D:91:ALA:C	2.54	0.45
1:C:24:SER:OG	1:C:59:ASP:OD2	2.24	0.45
1:C:90:GLN:HG3	1:C:197:LEU:HD12	1.99	0.44
1:D:225:ASP:C	1:D:225:ASP:OD1	2.55	0.44
1:B:60:THR:N	1:B:61:PRO:HD2	2.32	0.44
1:D:1:MET:HB2	1:D:103:LEU:CD1	2.48	0.44
1:A:243:GLU:HG2	1:A:249:LYS:HA	1.99	0.44
1:A:60:THR:CG2	1:A:64:GLN:NE2	2.81	0.44
1:D:90:GLN:HG3	1:D:197:LEU:HD12	1.99	0.44
1:B:174:GLY:HA2	1:B:176:TYR:CZ	2.53	0.44
1:B:275:LEU:O	1:B:281:GLY:HA3	2.18	0.44
1:A:16:LEU:HD12	1:A:25:LYS:HD2	1.99	0.44
1:D:17:HIS:HD2	1:D:20:THR:OG1	2.01	0.44
3:D:506:TRH:H2'2	3:D:506:TRH:O5'	2.18	0.44
1:C:35:MET:O	1:C:39:PRO:HD2	2.17	0.43
1:B:32:ASP:OD2	1:B:243:GLU:OE1	2.35	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:227:GLY:C	1:D:228:THR:CG2	2.85	0.43
1:D:14:THR:O	1:D:15:ARG:C	2.55	0.43
1:B:272:ALA:O	1:B:273:ALA:C	2.55	0.43
1:C:65:GLN:HE22	1:D:58:GLN:HE22	1.66	0.43
1:A:88:LEU:HD23	1:A:88:LEU:N	2.33	0.43
1:B:22:ALA:C	1:B:23:ILE:HG13	2.39	0.43
1:C:286:ARG:NH1	1:C:290:GLU:OE1	2.45	0.43
1:D:228:THR:O	1:D:229:HIS:C	2.57	0.43
1:B:60:THR:CB	1:B:61:PRO:HD3	2.49	0.42
1:C:87:GLY:HA2	3:C:504:TRH:HCA2	2.00	0.42
1:B:31:TYR:CD1	1:B:240:ALA:HB2	2.53	0.42
1:B:38:TYR:HB2	1:B:39:PRO:CD	2.49	0.42
1:C:24:SER:HB3	1:C:26:GLN:NE2	2.33	0.42
1:B:238:PHE:CE1	1:D:238:PHE:CE1	3.07	0.42
1:C:164:LEU:HA	1:C:164:LEU:HD23	1.93	0.42
1:D:192:SER:HB2	1:D:193:PRO:CD	2.50	0.42
1:C:192:SER:HB2	1:C:193:PRO:HD2	2.01	0.42
1:B:16:LEU:CD1	1:B:25:LYS:HD3	2.49	0.42
1:D:57:PRO:HA	1:D:81:VAL:HG22	2.01	0.42
1:D:84:SER:HA	1:D:85:PRO:HD3	1.93	0.42
1:A:90:GLN:HG3	1:A:197:LEU:HD12	2.01	0.42
1:C:237:GLN:HE22	1:D:237:GLN:HE21	1.68	0.42
1:B:273:ALA:HB3	1:B:274:PRO:CD	2.45	0.42
1:D:1:MET:N	1:D:129:GLN:NE2	2.66	0.42
1:C:35:MET:SD	1:C:110:ASP:HA	2.59	0.42
1:A:199:ILE:HD12	1:A:199:ILE:HA	1.89	0.42
1:A:138:HIS:ND1	1:C:246:GLN:O	2.47	0.42
1:B:286:ARG:NH1	1:B:290:GLU:OE1	2.52	0.41
1:C:11:GLY:HA3	3:C:504:TRH:C2'	2.49	0.41
1:D:60:THR:CG2	1:D:64:GLN:OE1	2.69	0.41
1:C:199:ILE:HA	1:C:199:ILE:HD12	1.91	0.41
1:C:58:GLN:HG2	1:C:58:GLN:O	2.20	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.77	0.41
1:B:26:GLN:HE21	1:B:26:GLN:HB2	1.55	0.41
1:A:146:GLY:HA2	1:A:161:GLU:HA	2.03	0.41
1:D:148:VAL:HG22	1:D:150:PHE:CE1	2.55	0.41
1:A:151:ASP:C	1:A:151:ASP:OD1	2.59	0.41
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.70	0.41
1:C:148:VAL:HB	1:C:159:LEU:HD23	2.02	0.41
1:D:199:ILE:HA	1:D:199:ILE:HD12	1.88	0.41
1:C:60:THR:N	1:C:61:PRO:CD	2.83	0.41
1:C:32:ASP:OD2	1:C:243:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:ARG:HD3	1:A:209:ARG:HH11	1.70	0.41
1:D:34:PRO:O	1:D:37:TYR:HB2	2.21	0.41
1:B:25:LYS:NZ	1:B:226:THR:O	2.46	0.40
1:C:243:GLU:HG2	1:C:249:LYS:HA	2.01	0.40
1:B:264:ASP:C	1:B:264:ASP:OD1	2.59	0.40
1:C:26:GLN:N	1:C:26:GLN:NE2	2.61	0.40
1:C:90:GLN:O	1:C:91:ALA:C	2.57	0.40
1:B:23:ILE:CD1	1:B:23:ILE:N	2.82	0.40
1:C:25:LYS:NZ	1:C:226:THR:O	2.49	0.40
1:C:65:GLN:HE22	1:D:58:GLN:NE2	2.20	0.40
1:D:147:VAL:HG12	1:D:148:VAL:N	2.37	0.40
1:C:17:HIS:HD2	1:C:20:THR:OG1	2.05	0.40
1:A:227:GLY:C	1:A:228:THR:CG2	2.87	0.40
1:B:54:ILE:HG21	1:B:54:ILE:HD13	1.83	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	290/293 (99%)	278 (96%)	11 (4%)	1 (0%)	50	82
1	B	290/293 (99%)	279 (96%)	9 (3%)	2 (1%)	30	62
1	C	290/293 (99%)	277 (96%)	9 (3%)	4 (1%)	16	41
1	D	291/293 (99%)	281 (97%)	9 (3%)	1 (0%)	50	82
All	All	1161/1172 (99%)	1115 (96%)	38 (3%)	8 (1%)	30	62

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	ARG
1	C	16	LEU
1	B	31	TYR
1	C	31	TYR

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Mol	Chain	Res	Type
1	A	31	TYR
1	B	16	LEU
1	C	12	SER
1	D	31	TYR

### 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	239/240 (100%)	228 (95%)	11 (5%)	37	70
1	B	239/240 (100%)	226 (95%)	13 (5%)	31	61
1	C	239/240 (100%)	232 (97%)	7 (3%)	55	85
1	D	240/240 (100%)	228 (95%)	12 (5%)	34	66
All	All	957/960 (100%)	914 (96%)	43 (4%)	38	70

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	THR
1	A	81	VAL
1	A	111	ASN
1	A	148	VAL
1	A	152	GLN
1	A	158	SER
1	A	160	GLU
1	A	168	SER
1	A	209	ARG
1	A	225	ASP
1	A	252	CYS
1	B	14	THR
1	B	23	ILE
1	B	26	GLN
1	B	60	THR
1	B	81	VAL
1	B	88	LEU
1	B	90	GLN

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Mol	Chain	Res	Type
1	B	126	SER
1	B	148	VAL
1	B	158	SER
1	B	209	ARG
1	B	225	ASP
1	B	252	CYS
1	C	14	THR
1	C	26	GLN
1	C	55	SER
1	C	60	THR
1	C	148	VAL
1	C	225	ASP
1	C	252	CYS
1	D	2	LYS
1	D	20	THR
1	D	23	ILE
1	D	26	GLN
1	D	60	THR
1	D	81	VAL
1	D	126	SER
1	D	148	VAL
1	D	168	SER
1	D	213	SER
1	D	225	ASP
1	D	252	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	B	17	HIS
1	B	26	GLN
1	B	58	GLN
1	B	116	HIS
1	C	17	HIS
1	C	26	GLN
1	C	58	GLN
1	C	65	GLN
1	D	17	HIS
1	D	26	GLN
1	D	129	GLN
1	D	237	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	TRH	A	500	-	37,37,37	1.86	9 (24%)	52,57,57	2.95	18 (34%)
3	TRH	A	501	-	37,37,37	1.56	7 (18%)	52,57,57	3.98	17 (32%)
2	SO4	A	701	-	4,4,4	0.61	0	6,6,6	0.67	0
3	TRH	B	502	-	37,37,37	1.63	8 (21%)	52,57,57	4.03	16 (30%)
3	TRH	B	503	-	37,37,37	1.49	8 (21%)	52,57,57	4.39	17 (32%)
2	SO4	B	700	-	4,4,4	0.59	0	6,6,6	0.68	0
2	SO4	B	702	-	4,4,4	0.23	0	6,6,6	0.59	0
3	TRH	C	504	-	37,37,37	1.67	8 (21%)	52,57,57	4.54	22 (42%)
3	TRH	C	505	-	37,37,37	1.73	7 (18%)	52,57,57	3.85	20 (38%)
2	SO4	C	703	-	4,4,4	0.19	0	6,6,6	0.66	0
3	TRH	D	506	-	37,37,37	1.46	6 (16%)	52,57,57	3.60	15 (28%)
3	TRH	D	507	-	37,37,37	1.60	9 (24%)	52,57,57	3.42	16 (30%)
2	SO4	D	704	-	4,4,4	0.40	0	6,6,6	0.61	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
3	TRH	A	500	-	-	0/18/53/53	0/3/3/3
3	TRH	A	501	-	-	0/18/53/53	0/3/3/3
2	SO4	A	701	-	-	0/0/0/0	0/0/0/0
3	TRH	B	502	-	-	0/18/53/53	0/3/3/3
3	TRH	B	503	-	-	0/18/53/53	0/3/3/3
2	SO4	B	700	-	-	0/0/0/0	0/0/0/0
2	SO4	B	702	-	-	0/0/0/0	0/0/0/0
3	TRH	C	504	-	-	0/18/53/53	0/3/3/3
3	TRH	C	505	-	-	0/18/53/53	0/3/3/3
2	SO4	C	703	-	-	0/0/0/0	0/0/0/0
3	TRH	D	506	-	-	0/18/53/53	0/3/3/3
3	TRH	D	507	-	-	0/18/53/53	0/3/3/3
2	SO4	D	704	-	-	0/0/0/0	0/0/0/0

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	TRH	O41-C41	5.55	1.35	1.24
3	A	500	TRH	O41-C41	5.16	1.34	1.24
3	A	500	TRH	C21-N11	-5.13	1.32	1.38
3	C	504	TRH	O41-C41	4.90	1.34	1.24
3	A	501	TRH	O21-C21	4.52	1.33	1.23
3	C	505	TRH	O21-C21	4.50	1.32	1.23
3	D	507	TRH	O21-C21	4.50	1.32	1.23
3	C	505	TRH	O41-C41	4.25	1.32	1.24
3	A	501	TRH	O41-C41	4.23	1.32	1.24
3	C	504	TRH	O21-C21	4.07	1.32	1.23
3	D	506	TRH	O41-C41	3.96	1.32	1.24
3	D	507	TRH	O41-C41	3.96	1.32	1.24
3	B	503	TRH	O21-C21	3.93	1.31	1.23
3	B	503	TRH	O41-C41	3.76	1.31	1.24
3	A	500	TRH	O5-C5	-3.68	1.35	1.44
3	A	500	TRH	O21-C21	3.63	1.31	1.23
3	B	502	TRH	O21-C21	3.62	1.31	1.23
3	D	506	TRH	O21-C21	3.59	1.31	1.23
3	C	504	TRH	C21-N11	-3.41	1.34	1.38
3	C	505	TRH	C41-C51	-3.02	1.36	1.42
3	C	505	TRH	O4'-C4'	-2.89	1.38	1.45
3	C	505	TRH	P2-O3P	2.87	1.62	1.51
3	A	500	TRH	C41-C51	-2.84	1.36	1.42
3	D	507	TRH	P2-O3P	2.84	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	TRH	C41-C51	-2.83	1.36	1.42
3	C	505	TRH	C21-N31	-2.75	1.32	1.37
3	B	502	TRH	C21-N11	-2.73	1.35	1.38
3	C	505	TRH	C21-N11	-2.72	1.35	1.38
3	D	507	TRH	C21-N31	-2.66	1.32	1.37
3	B	503	TRH	C41-C51	-2.66	1.36	1.42
3	D	507	TRH	P-O2P	2.63	1.61	1.51
3	C	504	TRH	C41-N31	-2.60	1.32	1.37
3	B	502	TRH	P-O2P	2.54	1.61	1.51
3	A	501	TRH	C41-N31	-2.47	1.33	1.37
3	C	504	TRH	P-O2P	2.46	1.60	1.51
3	B	502	TRH	P2-OPP	-2.46	1.55	1.59
3	C	504	TRH	P2-O3P	2.45	1.60	1.51
3	D	507	TRH	C41-C51	-2.42	1.37	1.42
3	D	507	TRH	C41-N31	-2.42	1.33	1.37
3	C	504	TRH	O4'-C4'	-2.41	1.39	1.45
3	A	501	TRH	P-O2P	2.39	1.60	1.51
3	D	507	TRH	C21-N11	-2.39	1.35	1.38
3	A	500	TRH	P2-O3P	2.38	1.60	1.51
3	B	503	TRH	P-O2P	2.37	1.60	1.51
3	B	503	TRH	C21-N11	-2.36	1.35	1.38
3	A	501	TRH	C41-C51	-2.36	1.37	1.42
3	D	506	TRH	C41-C51	-2.33	1.37	1.42
3	D	506	TRH	C2'-C3'	-2.30	1.46	1.52
3	B	502	TRH	C21-N31	-2.24	1.33	1.37
3	B	502	TRH	P2-O3P	2.20	1.59	1.51
3	D	506	TRH	O4'-C4'	-2.20	1.39	1.45
3	A	500	TRH	O4'-C4'	-2.17	1.39	1.45
3	D	506	TRH	C21-N31	-2.17	1.33	1.37
3	B	503	TRH	O4'-C4'	-2.17	1.40	1.45
3	A	501	TRH	P2-O3P	2.16	1.59	1.51
3	B	503	TRH	C41-N31	-2.15	1.33	1.37
3	C	504	TRH	P-OPP	2.05	1.63	1.59
3	A	500	TRH	O1-C1	2.05	1.45	1.42
3	A	501	TRH	C21-N31	-2.04	1.33	1.37
3	B	503	TRH	C3'-C4'	-2.04	1.47	1.53
3	D	507	TRH	O4'-C4'	-2.03	1.40	1.45
3	A	500	TRH	P-O2P	2.01	1.59	1.51

All (141) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	TRH	O5-C1-O1	-18.69	86.94	111.36
3	B	502	TRH	O5-C1-O1	-18.31	87.43	111.36
3	C	505	TRH	O5-C1-O1	-17.92	87.94	111.36
3	A	501	TRH	O5-C1-O1	-16.41	89.92	111.36
3	C	504	TRH	O5-C1-O1	-16.31	90.05	111.36
3	D	506	TRH	O5-C1-O1	-15.95	90.52	111.36
3	D	507	TRH	O5-C1-O1	-14.67	92.19	111.36
3	C	504	TRH	C61-N11-C21	-14.47	118.30	122.41
3	C	504	TRH	C1-O5-C5	-14.21	89.90	113.55
3	C	505	TRH	C1-O5-C5	-13.90	90.42	113.55
3	B	503	TRH	C61-N11-C21	-13.54	118.56	122.41
3	B	503	TRH	C1-O5-C5	-12.33	93.02	113.55
3	D	507	TRH	C1-O5-C5	-12.22	93.22	113.55
3	B	502	TRH	C61-N11-C21	-12.12	118.97	122.41
3	A	501	TRH	C61-N11-C21	-11.64	119.10	122.41
3	A	501	TRH	C1-O5-C5	-11.57	94.29	113.55
3	B	502	TRH	C1-O5-C5	-11.52	94.37	113.55
3	A	500	TRH	O5-C1-O1	10.77	125.44	111.36
3	D	506	TRH	C1-O5-C5	-9.97	96.96	113.55
3	B	503	TRH	O4'-C1'-C2'	-8.77	88.97	106.25
3	C	504	TRH	O4'-C1'-N11	8.65	123.94	107.68
3	C	504	TRH	N31-C21-N11	8.54	123.10	115.97
3	D	507	TRH	O4'-C1'-C2'	-8.37	89.76	106.25
3	D	506	TRH	O4'-C1'-C2'	-8.25	89.98	106.25
3	D	506	TRH	C61-N11-C21	-8.15	120.09	122.41
3	B	502	TRH	O4'-C1'-C2'	-8.05	90.39	106.25
3	A	500	TRH	O5-C5-C4	-7.91	96.17	109.53
3	B	503	TRH	N31-C21-N11	7.67	122.38	115.97
3	A	501	TRH	N31-C21-N11	7.29	122.05	115.97
3	D	506	TRH	N31-C21-N11	7.02	121.83	115.97
3	B	502	TRH	N31-C21-N11	6.77	121.62	115.97
3	A	501	TRH	O4'-C1'-C2'	-6.72	93.00	106.25
3	A	500	TRH	N31-C21-N11	5.85	120.85	115.97
3	A	500	TRH	O4'-C1'-C2'	-5.64	95.13	106.25
3	C	504	TRH	C4'-O4'-C1'	5.61	123.64	109.44
3	A	501	TRH	C4'-O4'-C1'	5.61	123.64	109.44
3	A	501	TRH	C6-C5-C4	-5.48	104.17	113.06
3	C	505	TRH	O4'-C1'-C2'	-5.40	95.61	106.25
3	B	503	TRH	C6-C5-C4	-5.40	104.30	113.06
3	C	505	TRH	C6-C5-C4	-5.31	104.43	113.06
3	C	504	TRH	O4'-C1'-C2'	-5.30	95.81	106.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	TRH	C4'-O4'-C1'	5.22	122.67	109.44
3	C	505	TRH	O5-C5-C6	4.98	117.69	106.70
3	C	504	TRH	O1-C1-C2	4.98	117.50	108.38
3	A	500	TRH	C6-C5-C4	4.80	120.86	113.06
3	C	505	TRH	N31-C21-N11	4.63	119.84	115.97
3	B	503	TRH	C4-C3-C2	-4.63	102.26	110.82
3	D	507	TRH	N31-C21-N11	4.62	119.83	115.97
3	A	500	TRH	O5-C1-C2	-4.52	101.05	110.31
3	A	500	TRH	C1-O5-C5	4.46	120.98	113.55
3	A	501	TRH	O4'-C1'-N11	4.42	115.99	107.68
3	D	506	TRH	O4'-C4'-C5'	-4.31	93.99	109.36
3	C	504	TRH	C6-C5-C4	-4.23	106.19	113.06
3	A	501	TRH	C5A-C51-C41	-4.23	116.72	121.04
3	A	500	TRH	C4'-O4'-C1'	4.19	120.05	109.44
3	C	504	TRH	O5-C5-C6	4.18	115.92	106.70
3	C	505	TRH	C4'-O4'-C1'	4.16	119.99	109.44
3	C	505	TRH	C4-C3-C2	-4.13	103.18	110.82
3	C	504	TRH	P-OPP-P2	-4.06	119.78	131.68
3	B	502	TRH	O5-C5-C6	3.86	115.22	106.70
3	D	507	TRH	O4'-C1'-N11	3.86	114.93	107.68
3	B	502	TRH	C4'-O4'-C1'	3.82	119.12	109.44
3	D	507	TRH	C51-C61-N11	-3.79	117.90	121.59
3	D	506	TRH	O4'-C1'-N11	3.74	114.72	107.68
3	B	503	TRH	O4'-C1'-N11	3.69	114.61	107.68
3	D	507	TRH	C4'-O4'-C1'	3.65	118.67	109.44
3	A	500	TRH	O4'-C4'-C5'	-3.62	96.42	109.36
3	D	506	TRH	C4'-O4'-C1'	3.60	118.57	109.44
3	A	500	TRH	C51-C61-N11	-3.34	118.33	121.59
3	D	507	TRH	O4-C4-C3	-3.34	102.87	110.35
3	C	504	TRH	O4'-C4'-C3'	-3.33	97.21	105.66
3	C	505	TRH	P-OPP-P2	-3.31	121.97	131.68
3	D	507	TRH	O5-C5-C6	3.31	114.00	106.70
3	D	507	TRH	O4'-C4'-C3'	-3.30	97.29	105.66
3	B	503	TRH	O5-C5-C6	3.26	113.88	106.70
3	D	506	TRH	O4-C4-C5	3.21	117.21	109.78
3	D	507	TRH	O4'-C4'-C5'	-3.20	97.94	109.36
3	A	500	TRH	O4-C4-C5	-3.19	102.39	109.78
3	A	500	TRH	C41-N31-C21	-3.19	118.85	125.39
3	A	500	TRH	P2-O1-C1	3.16	132.93	119.58
3	B	502	TRH	P-OPP-P2	-3.14	122.47	131.68
3	C	505	TRH	O3-C3-C4	-3.13	103.33	110.35
3	A	501	TRH	C51-C61-N11	-3.07	118.60	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	506	TRH	C41-N31-C21	-3.01	119.22	125.39
3	B	503	TRH	P-OPP-P2	-2.99	122.92	131.68
3	C	505	TRH	O5'-C5'-C4'	-2.95	98.11	108.94
3	B	503	TRH	O5'-P-O2P	-2.92	97.93	109.37
3	D	507	TRH	P-OPP-P2	-2.90	123.19	131.68
3	C	505	TRH	C41-N31-C21	-2.89	119.45	125.39
3	C	504	TRH	O5-C1-C2	2.87	116.20	110.31
3	C	504	TRH	C4-C3-C2	-2.85	105.56	110.82
3	B	503	TRH	C41-N31-C21	-2.83	119.58	125.39
3	C	504	TRH	C3'-C2'-C1'	2.80	109.93	102.47
3	D	506	TRH	P-OPP-P2	-2.78	123.53	131.68
3	A	501	TRH	O5-C5-C6	2.77	112.82	106.70
3	C	505	TRH	C51-C61-N11	-2.75	118.91	121.59
3	C	505	TRH	O4'-C4'-C5'	-2.75	99.55	109.36
3	B	503	TRH	O4'-C4'-C5'	-2.73	99.61	109.36
3	D	507	TRH	O2-C2-C1	-2.68	104.20	110.04
3	B	502	TRH	O1-C1-C2	2.66	113.25	108.38
3	D	506	TRH	C51-C61-N11	-2.64	119.02	121.59
3	B	503	TRH	O5-C5-C4	2.63	113.97	109.53
3	A	501	TRH	C41-N31-C21	-2.62	120.01	125.39
3	D	506	TRH	O5-C5-C6	2.60	112.44	106.70
3	B	502	TRH	C41-N31-C21	-2.58	120.09	125.39
3	D	507	TRH	C41-N31-C21	-2.55	120.16	125.39
3	C	505	TRH	O1P-P-O2P	2.54	126.42	112.21
3	C	504	TRH	C61-N11-C1'	2.48	125.48	119.33
3	D	506	TRH	C2'-C1'-N11	-2.45	107.71	114.08
3	B	502	TRH	O3-C3-C4	-2.42	104.93	110.35
3	B	502	TRH	C3'-C2'-C1'	2.40	108.88	102.47
3	A	501	TRH	P-OPP-P2	-2.40	124.64	131.68
3	D	506	TRH	O4'-C4'-C3'	-2.38	99.63	105.66
3	C	505	TRH	O2-C2-C3	-2.36	105.06	110.35
3	A	500	TRH	O4'-C4'-C3'	-2.34	99.72	105.66
3	B	502	TRH	O4'-C4'-C5'	-2.34	101.01	109.36
3	B	503	TRH	O4'-C4'-C3'	-2.29	99.84	105.66
3	C	505	TRH	O4-C4-C5	2.28	115.05	109.78
3	B	503	TRH	O2-C2-C3	-2.28	105.25	110.35
3	C	504	TRH	C2'-C3'-C4'	2.27	107.82	102.73
3	A	501	TRH	O5-C5-C4	2.27	113.36	109.53
3	C	505	TRH	O4'-C4'-C3'	-2.27	99.92	105.66
3	D	507	TRH	C5A-C51-C41	-2.26	118.74	121.04
3	A	501	TRH	C61-C51-C41	2.26	120.58	115.11
3	C	504	TRH	C41-N31-C21	-2.24	120.78	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	504	TRH	C51-C61-N11	-2.24	119.41	121.59
3	B	502	TRH	O1P-P-O2P	2.24	124.72	112.21
3	C	505	TRH	O5'-P-O2P	-2.22	100.67	109.37
3	D	507	TRH	O4-C4-C5	2.22	114.91	109.78
3	B	502	TRH	OPP-P-O5'	-2.22	93.49	103.41
3	C	504	TRH	O3-C3-C4	-2.20	105.42	110.35
3	B	502	TRH	O4'-C4'-C3'	-2.19	100.11	105.66
3	A	500	TRH	O5-C5-C6	-2.18	101.89	106.70
3	A	501	TRH	C3'-C2'-C1'	2.13	108.16	102.47
3	A	501	TRH	O4'-C4'-C3'	-2.13	100.26	105.66
3	A	500	TRH	O1P-P-O2P	2.12	124.05	112.21
3	C	504	TRH	O3-C3-C2	2.12	115.10	110.35
3	C	504	TRH	OPP-P2-O1	-2.07	98.26	103.48
3	C	505	TRH	O4-C4-C3	-2.06	105.74	110.35
3	A	500	TRH	C4-C3-C2	2.03	114.58	110.82
3	A	500	TRH	P-OPP-P2	-2.01	125.78	131.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	292/293 (99%)	-0.39	1 (0%) 91 95	6, 11, 21, 34	0
1	B	292/293 (99%)	-0.37	2 (0%) 84 89	7, 12, 22, 33	0
1	C	292/293 (99%)	-0.28	2 (0%) 84 89	6, 13, 23, 35	0
1	D	293/293 (100%)	-0.30	2 (0%) 84 89	7, 11, 22, 36	0
All	All	1169/1172 (99%)	-0.33	7 (0%) 83 90	6, 11, 22, 36	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.9
1	A	13	GLY	2.6
1	B	15	ARG	2.4
1	B	152	GLN	2.2
1	C	152	GLN	2.2
1	C	101	ASN	2.1
1	D	13	GLY	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	D	704	5/5	0.46	6.66	43,44,45,46	0
2	SO4	C	703	5/5	0.47	3.60	41,44,46,46	0
2	SO4	B	700	5/5	0.21	3.12	42,42,45,46	0
3	TRH	C	505	35/35	0.16	0.90	8,12,15,17	0
2	SO4	B	702	5/5	0.26	0.81	41,42,46,47	0
3	TRH	D	507	35/35	0.15	0.79	7,14,20,22	0
2	SO4	A	701	5/5	0.19	0.32	38,40,41,42	0
3	TRH	B	502	35/35	0.15	-0.11	8,12,16,20	0
3	TRH	C	504	35/35	0.15	-0.19	9,13,18,21	0
3	TRH	B	503	35/35	0.14	-0.22	8,13,16,19	0
3	TRH	D	506	35/35	0.13	-0.25	8,14,18,18	0
3	TRH	A	500	35/35	0.13	-0.33	6,11,14,19	0
3	TRH	A	501	35/35	0.14	-0.36	7,10,17,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.