



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 29, 2021 – 04:15 PM JST

PDB ID : 7CLL  
Title : Mycobacterium tuberculosis enolase in complex with 2-Phosphoglycerate  
Authors : Ahmad, M.; Jha, B.; Tiwari, S.; Pal, R.K.; Biswal, B.K.  
Deposited on : 2020-07-21  
Resolution : 1.99 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 : 2.22  
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) : 2.22

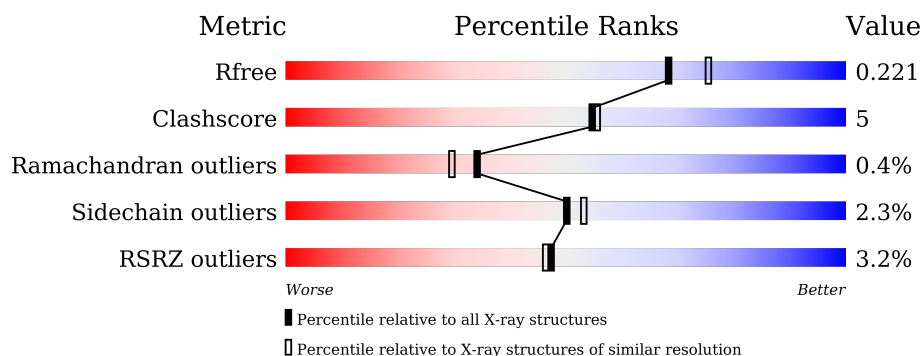
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	436	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	436	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	436	<div> <div></div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	436	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	505	-	-	X	-
5	ACT	D	504	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13697 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 Enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	1	0
			3082	1935	534	606	7			
1	B	424	Total	C	N	O	S	0	1	0
			3114	1949	541	617	7			
1	C	426	Total	C	N	O	S	0	1	0
			3136	1965	540	623	8			
1	D	424	Total	C	N	O	S	0	1	0
			3115	1953	540	615	7			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A0E8NV14
A	-5	HIS	-	expression tag	UNP A0A0E8NV14
A	-4	HIS	-	expression tag	UNP A0A0E8NV14
A	-3	HIS	-	expression tag	UNP A0A0E8NV14
A	-2	HIS	-	expression tag	UNP A0A0E8NV14
A	-1	HIS	-	expression tag	UNP A0A0E8NV14
A	0	HIS	-	expression tag	UNP A0A0E8NV14
B	-6	MET	-	initiating methionine	UNP A0A0E8NV14
B	-5	HIS	-	expression tag	UNP A0A0E8NV14
B	-4	HIS	-	expression tag	UNP A0A0E8NV14
B	-3	HIS	-	expression tag	UNP A0A0E8NV14
B	-2	HIS	-	expression tag	UNP A0A0E8NV14
B	-1	HIS	-	expression tag	UNP A0A0E8NV14
B	0	HIS	-	expression tag	UNP A0A0E8NV14
C	-6	MET	-	initiating methionine	UNP A0A0E8NV14
C	-5	HIS	-	expression tag	UNP A0A0E8NV14
C	-4	HIS	-	expression tag	UNP A0A0E8NV14
C	-3	HIS	-	expression tag	UNP A0A0E8NV14
C	-2	HIS	-	expression tag	UNP A0A0E8NV14
C	-1	HIS	-	expression tag	UNP A0A0E8NV14
C	0	HIS	-	expression tag	UNP A0A0E8NV14

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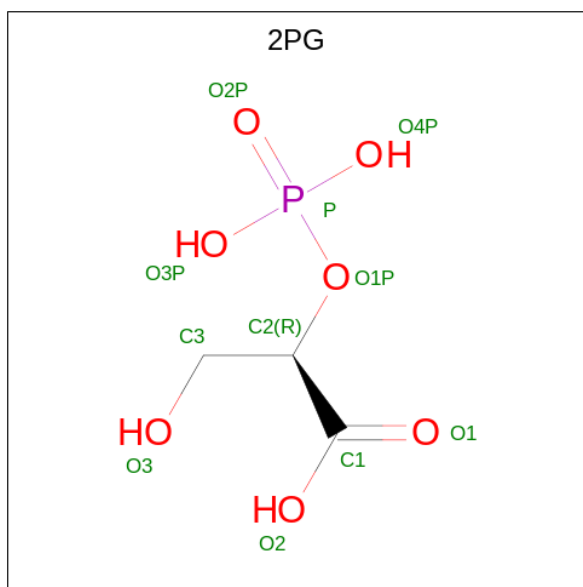
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP A0A0E8NV14
D	-5	HIS	-	expression tag	UNP A0A0E8NV14
D	-4	HIS	-	expression tag	UNP A0A0E8NV14
D	-3	HIS	-	expression tag	UNP A0A0E8NV14
D	-2	HIS	-	expression tag	UNP A0A0E8NV14
D	-1	HIS	-	expression tag	UNP A0A0E8NV14
D	0	HIS	-	expression tag	UNP A0A0E8NV14

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0

- Molecule 3 is 2-PHOSPHOGLYCERIC ACID (three-letter code: 2PG) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>7</sub>P).



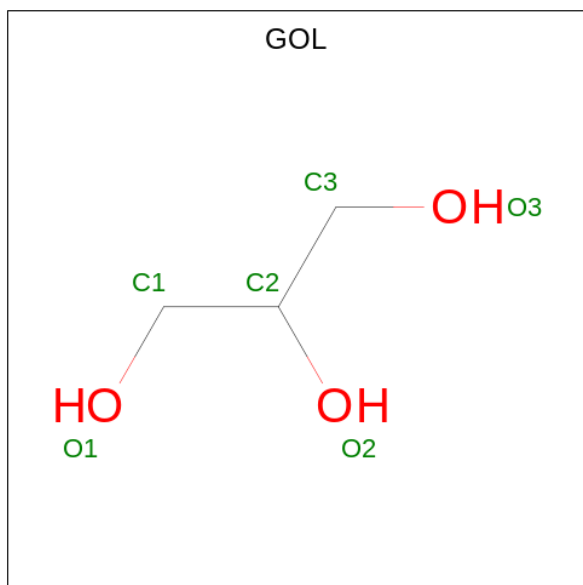
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 11 3 7 1	0	0

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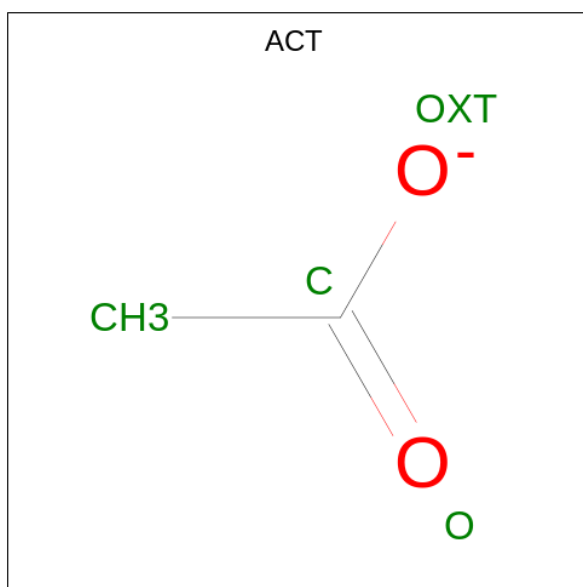
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			11	3	7	1		
3	C	1	Total	C	O	P	0	0
			11	3	7	1		
3	D	1	Total	C	O	P	0	0
			11	3	7	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		
6	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Cl	0	0
			1	1		

- Molecule 8 is water.

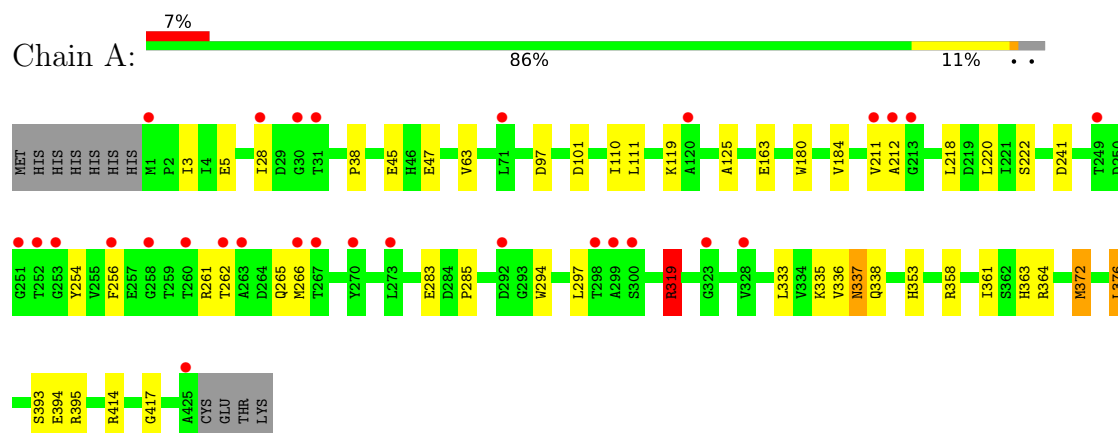
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	210	Total	O	0	0
			210	210		
8	B	261	Total	O	0	0
			261	261		
8	C	369	Total	O	0	0
			369	369		
8	D	301	Total	O	0	0
			301	301		



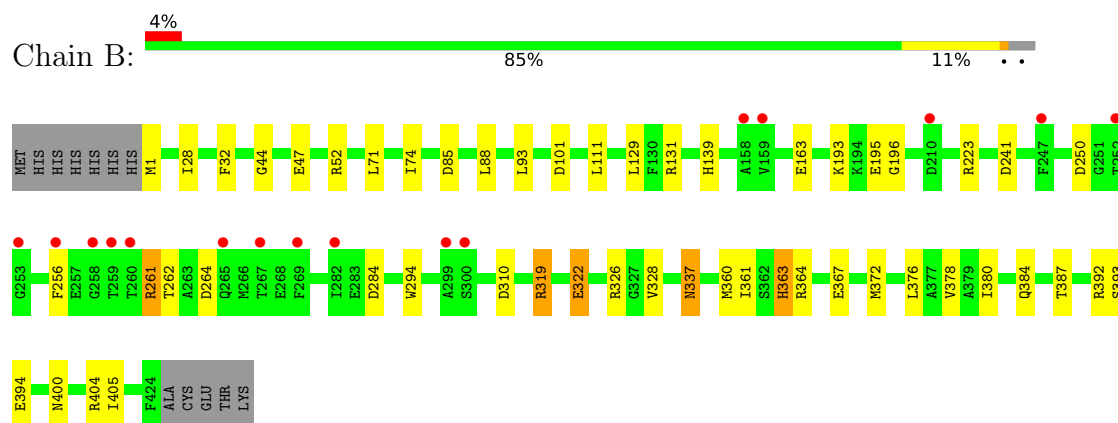
### 3 Residue-property plots [i](#)

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

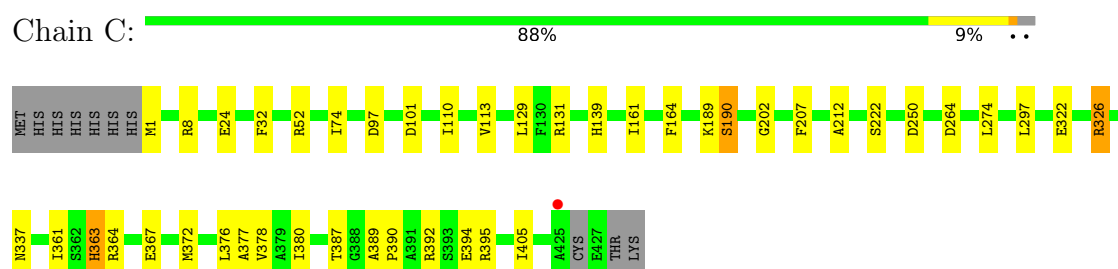
#### • Molecule 1: Enolase



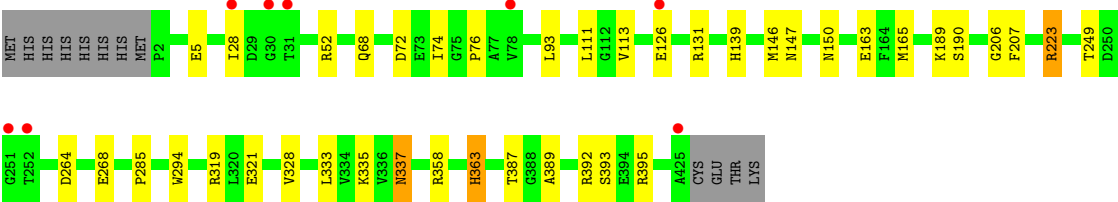
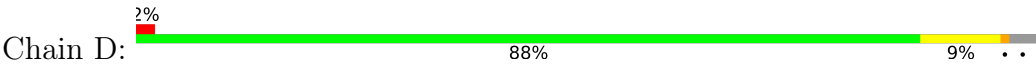
#### • Molecule 1: Enolase



#### • Molecule 1: Enolase



● Molecule 1: Enolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.70Å 197.32Å 200.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 1.99 49.33 – 1.99	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.38-1.99) 91.2 (49.33-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.175 , 0.221 0.175 , 0.221	Depositor DCC
$R_{free}$ test set	5913 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.79% 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: GOL, PEG, 2PG, ACT, CL, MG

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	0.60	0/3135	0.74	0/4268
1	B	0.66	0/3168	0.79	2/4309 (0.0%)
1	C	0.74	0/3189	0.84	0/4336
1	D	0.71	0/3169	0.80	0/4310
All	All	0.68	0/12661	0.79	2/17223 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	195	GLU	C-N-CA	-5.64	110.46	122.30
1	B	131	ARG	CB-CA-C	5.38	121.16	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	414	ARG	Sidechain
1	B	196	GLY	Peptide
1	B	319	ARG	Sidechain
1	B	52	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	326	ARG	Sidechain
1	C	395	ARG	Sidechain
1	C	52	ARG	Sidechain
1	D	223	ARG	Sidechain
1	D	319	ARG	Sidechain
1	D	395	ARG	Sidechain
1	D	52	ARG	Sidechain

## 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	3082	0	3010	47	1
1	B	3114	0	3056	35	0
1	C	3136	0	3088	30	0
1	D	3115	0	3066	20	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	11	0	4	1	0
3	B	11	0	4	0	0
3	C	11	0	4	0	0
3	D	11	0	4	0	0
4	A	6	0	8	0	0
4	C	12	0	16	0	0
5	A	4	0	3	0	0
5	B	8	0	6	4	0
5	C	8	0	6	0	0
5	D	4	0	3	2	0
6	C	7	0	10	1	0
6	D	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	1	0	0	0	0
8	A	210	0	0	8	0
8	B	261	0	0	4	0
8	C	369	0	0	9	0
8	D	301	0	0	3	0
All	All	13697	0	12298	130	1

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 (130) 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:119:LYS:HE3	1:A:372[A]:MET:CE	1.70	1.22
1:A:119:LYS:CE	1:A:372[A]:MET:HE2	1.78	1.13
1:B:372[B]:MET:HE2	1:B:376:LEU:HD13	1.11	1.08
1:B:223:ARG:HH11	5:B:505:ACT:H2	1.07	1.08
1:B:361:ILE:HD11	1:B:380:ILE:HD11	1.04	1.02
1:B:361:ILE:HD11	1:B:380:ILE:CD1	1.93	0.99
1:B:372[B]:MET:CE	1:B:376:LEU:HD13	1.93	0.97
1:B:223:ARG:HH11	5:B:505:ACT:CH3	1.77	0.96
1:A:119:LYS:HE2	1:A:372[A]:MET:HE2	1.48	0.92
1:A:119:LYS:HE3	1:A:372[A]:MET:HE1	1.49	0.91
1:C:372[B]:MET:HE1	1:C:376:LEU:HD22	1.52	0.90
1:B:361:ILE:CD1	1:B:380:ILE:HD11	1.98	0.90
1:B:372[B]:MET:HE2	1:B:376:LEU:CD1	2.03	0.85
1:B:223:ARG:NH1	5:B:505:ACT:H2	1.90	0.84
1:A:119:LYS:CE	1:A:372[A]:MET:CE	2.45	0.82
1:C:372[B]:MET:CE	1:C:376:LEU:HD22	2.11	0.80
1:D:223:ARG:HD2	5:D:504:ACT:O	1.84	0.77
1:C:361:ILE:HD11	1:C:380:ILE:CD1	2.17	0.74
1:A:256:PHE:HB3	1:A:266:MET:HE1	1.68	0.74
1:B:71:LEU:HB2	8:B:816:HOH:O	1.89	0.71
1:C:361:ILE:HD11	1:C:380:ILE:HD11	1.73	0.70
1:A:285:PRO:HD2	1:A:294:TRP:CH2	2.25	0.70
1:C:74:ILE:HG21	1:C:113:VAL:HG21	1.78	0.66
1:A:335:LYS:NZ	8:A:602:HOH:O	2.31	0.62
1:A:262:THR:HG23	1:A:265:GLN:H	1.67	0.59
1:B:163:GLU:HB2	1:B:241:ASP:HB3	1.85	0.58
1:C:361:ILE:HD11	1:C:380:ILE:HD13	1.86	0.58
1:B:284:ASP:OD2	1:B:310:ASP:HB3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:HB3	1:A:266:MET:CE	2.35	0.57
1:B:1:MET:HB3	1:B:28:ILE:HD11	1.87	0.56
1:A:261:ARG:HA	1:A:265:GLN:OE1	2.05	0.56
1:C:101:ASP:HB3	8:C:930:HOH:O	2.05	0.56
1:C:129:LEU:HD21	1:C:372[A]:MET:HG3	1.86	0.56
1:A:256:PHE:CB	1:A:266:MET:HE1	2.35	0.54
1:A:212:ALA:N	8:A:603:HOH:O	2.35	0.54
1:B:361:ILE:HD12	1:B:361:ILE:N	2.23	0.54
1:A:297:LEU:C	1:A:297:LEU:HD23	2.29	0.54
1:C:24:GLU:CD	1:C:32:PHE:HZ	2.11	0.54
1:A:262:THR:CG2	1:A:265:GLN:HG3	2.38	0.53
1:B:256:PHE:O	1:B:261:ARG:NH2	2.41	0.53
1:D:223:ARG:CD	5:D:504:ACT:O	2.56	0.53
1:B:74:ILE:HG23	1:B:93:LEU:CD2	2.38	0.53
1:A:333:LEU:HD23	1:A:335:LYS:HE3	1.91	0.53
1:D:131:ARG:HD3	8:D:812:HOH:O	2.08	0.52
1:B:101:ASP:HB3	8:B:827:HOH:O	2.09	0.52
1:C:394:GLU:HB3	1:D:393:SER:HB2	1.92	0.51
1:C:129:LEU:CD2	1:C:372[A]:MET:HG3	2.40	0.51
1:D:285:PRO:HD2	1:D:294:TRP:CH2	2.45	0.51
1:A:262:THR:HG22	1:A:265:GLN:HG3	1.93	0.50
1:C:161:ILE:HB	1:C:164:PHE:CZ	2.46	0.50
1:C:364:ARG:O	1:C:367:GLU:HG2	2.10	0.50
1:A:125:ALA:HB1	8:A:635:HOH:O	2.11	0.50
1:A:333:LEU:CD2	1:A:335:LYS:HE3	2.41	0.50
1:D:150:ASN:ND2	1:D:206:GLY:HA3	2.27	0.50
1:C:322:GLU:OE2	1:C:326:ARG:HD2	2.12	0.50
1:B:322:GLU:OE1	1:B:326:ARG:HD2	2.12	0.50
1:D:147:ASN:CG	1:D:163:GLU:HB3	2.32	0.49
1:C:274:LEU:O	8:C:601:HOH:O	2.20	0.49
1:C:24:GLU:CD	1:C:32:PHE:CZ	2.87	0.48
1:A:254:TYR:HB3	1:A:266:MET:HE2	1.94	0.48
1:D:294:TRP:HB3	1:D:328:VAL:HG13	1.94	0.48
1:A:262:THR:HG22	1:A:265:GLN:CG	2.44	0.47
6:C:507:PEG:H32	8:C:943:HOH:O	2.13	0.47
1:B:44:GLY:O	1:B:47:GLU:HG3	2.15	0.47
1:C:190:SER:HB3	8:C:731:HOH:O	2.13	0.47
1:D:147:ASN:O	1:D:389:ALA:HB2	2.15	0.47
1:A:101:ASP:HB2	8:A:726:HOH:O	2.15	0.47
1:D:189:LYS:HB2	1:D:207:PHE:CZ	2.49	0.47
1:C:361:ILE:HG13	1:C:377:ALA:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:SER:HB2	1:B:394:GLU:HB3	1.98	0.46
1:A:361:ILE:HD11	1:A:376:LEU:HD23	1.98	0.46
1:A:211:VAL:HA	8:A:603:HOH:O	2.15	0.46
1:B:294:TRP:HB3	1:B:328:VAL:HG13	1.97	0.46
1:D:74:ILE:HG21	1:D:113:VAL:HG21	1.97	0.46
1:A:254:TYR:HB3	1:A:266:MET:HE3	1.98	0.46
1:B:193:LYS:HE2	1:B:193:LYS:HB2	1.52	0.46
1:C:326:ARG:NH1	8:C:617:HOH:O	2.49	0.45
1:A:336:VAL:HG21	1:A:372[B]:MET:CE	2.46	0.45
1:D:363:HIS:CG	1:D:387:THR:HA	2.51	0.45
1:A:256:PHE:CB	1:A:266:MET:CE	2.95	0.45
1:A:180:TRP:O	1:A:184:VAL:HG23	2.16	0.45
1:B:85:ASP:HB3	1:B:88:LEU:HB2	1.99	0.45
1:D:28:ILE:HD11	8:D:849:HOH:O	2.16	0.45
1:B:364:ARG:O	1:B:367:GLU:HG2	2.17	0.44
1:C:97:ASP:HB2	1:C:110:ILE:HD11	2.00	0.44
1:D:5:GLU:OE2	1:D:28:ILE:HD13	2.18	0.44
1:D:268:GLU:CB	8:D:886:HOH:O	2.65	0.44
1:C:297:LEU:C	1:C:297:LEU:HD23	2.37	0.44
1:A:63:VAL:HA	8:A:685:HOH:O	2.17	0.44
1:B:360:MET:HG3	1:B:384:GLN:HB3	2.00	0.44
1:A:319:ARG:HE	1:A:319:ARG:HB3	1.60	0.44
1:A:394:GLU:HB3	1:B:393:SER:HB2	2.00	0.44
1:B:262:THR:HB	8:B:605:HOH:O	2.18	0.44
1:D:111:LEU:HD22	1:D:337:ASN:HA	2.00	0.44
1:D:146:MET:O	1:D:165:MET:HA	2.18	0.43
1:A:5:GLU:HB2	1:A:28:ILE:HG23	1.99	0.43
1:A:361:ILE:CD1	1:A:376:LEU:HD23	2.49	0.43
1:B:264:ASP:HB2	8:B:607:HOH:O	2.17	0.43
1:A:283:GLU:OE2	1:A:333:LEU:HD22	2.18	0.43
1:C:378:VAL:HG21	1:C:405:ILE:HG21	2.01	0.43
1:D:74:ILE:HG23	1:D:93:LEU:CD2	2.49	0.43
1:A:47:GLU:CD	1:A:338:GLN:HG2	2.39	0.43
1:C:8:ARG:CG	8:C:861:HOH:O	2.67	0.43
1:C:101:ASP:HB3	8:C:915:HOH:O	2.19	0.42
1:A:3:ILE:HB	1:A:28:ILE:HG12	2.01	0.42
1:A:45:GLU:HA	8:A:770:HOH:O	2.18	0.42
1:D:333:LEU:HD23	1:D:335:LYS:HE3	2.00	0.42
1:A:111:LEU:HD22	1:A:337:ASN:HA	2.01	0.42
1:B:129:LEU:HD21	1:B:372[A]:MET:HG3	2.01	0.42
1:A:358:ARG:NH1	8:A:616:HOH:O	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:GLN:NE2	1:D:72:ASP:OD1	2.53	0.42
1:B:363:HIS:CG	1:B:387:THR:HA	2.55	0.42
1:A:241:ASP:HA	1:A:283:GLU:HB3	2.00	0.41
1:A:372[A]:MET:HE2	1:A:372[A]:MET:HB2	1.65	0.41
1:A:211:VAL:HG11	1:A:220:LEU:CD1	2.50	0.41
1:C:212:ALA:HB3	8:C:955:HOH:O	2.20	0.41
1:C:389:ALA:HB1	1:C:390:PRO:HD2	2.03	0.41
1:A:163:GLU:OE2	3:A:503:2PG:O3	2.31	0.41
1:B:400:ASN:O	1:B:404:ARG:HG3	2.20	0.41
1:A:38:PRO:HB2	1:A:364:ARG:HB2	2.02	0.41
1:B:129:LEU:HD21	1:B:372[A]:MET:CE	2.50	0.41
1:B:223:ARG:NH1	5:B:505:ACT:CH3	2.62	0.41
1:C:363:HIS:CG	1:C:387:THR:HA	2.56	0.41
1:B:111:LEU:HD22	1:B:337:ASN:HA	2.03	0.41
1:B:378:VAL:HG21	1:B:405:ILE:HG21	2.02	0.41
1:C:361:ILE:CD1	1:C:380:ILE:HD11	2.46	0.41
1:C:202:GLY:HA2	8:C:772:HOH:O	2.20	0.40
1:A:97:ASP:HB2	1:A:110:ILE:HD11	2.03	0.40
1:A:218:LEU:O	1:A:222:SER:HB2	2.21	0.40
1:C:189:LYS:HB2	1:C:207:PHE:CZ	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:HIS:O	1:A:353:HIS:O[3_455]	1.94	0.26

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	424/436 (97%)	403 (95%)	20 (5%)	1 (0%)	47 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	423/436 (97%)	405 (96%)	16 (4%)	2 (0%)	29	23
1	C	424/436 (97%)	406 (96%)	16 (4%)	2 (0%)	29	23
1	D	423/436 (97%)	409 (97%)	12 (3%)	2 (0%)	29	23
All	All	1694/1744 (97%)	1623 (96%)	64 (4%)	7 (0%)	34	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	139	HIS
1	D	139	HIS
1	B	139	HIS
1	C	392	ARG
1	A	417	GLY
1	B	392	ARG
1	D	392	ARG

### 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	301/326 (92%)	295 (98%)	6 (2%)	55	58
1	B	310/326 (95%)	303 (98%)	7 (2%)	50	53
1	C	314/326 (96%)	307 (98%)	7 (2%)	52	55
1	D	310/326 (95%)	301 (97%)	9 (3%)	42	43
All	All	1235/1304 (95%)	1206 (98%)	29 (2%)	50	53

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	A	337	ASN
1	A	363	HIS
1	A	372[A]	MET

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Mol	Chain	Res	Type
1	A	372[B]	MET
1	A	376	LEU
1	B	32	PHE
1	B	250	ASP
1	B	261	ARG
1	B	319	ARG
1	B	322	GLU
1	B	337	ASN
1	B	363	HIS
1	C	1	MET
1	C	190	SER
1	C	222	SER
1	C	250	ASP
1	C	264	ASP
1	C	337	ASN
1	C	363	HIS
1	D	76	PRO
1	D	126	GLU
1	D	190	SER
1	D	249	THR
1	D	264	ASP
1	D	321	GLU
1	D	337	ASN
1	D	358	ARG
1	D	363	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	B	150	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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
3	2PG	A	503	2	7,10,10	1.05	1 (14%)	8,14,14	1.41	1 (12%)
5	ACT	C	506	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
5	ACT	D	504	-	1,3,3	2.43	1 (100%)	0,3,3	0.00	-
3	2PG	D	503	2	7,10,10	1.20	1 (14%)	8,14,14	1.69	2 (25%)
5	ACT	A	505	-	1,3,3	2.11	1 (100%)	0,3,3	0.00	-
4	GOL	C	508	-	5,5,5	0.29	0	5,5,5	0.68	0
6	PEG	C	507	-	6,6,6	0.43	0	5,5,5	0.46	0
5	ACT	B	504	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
3	2PG	B	503	2	7,10,10	0.95	0	8,14,14	1.26	0
5	ACT	C	505	-	1,3,3	2.40	1 (100%)	0,3,3	0.00	-
6	PEG	D	505	-	6,6,6	0.60	0	5,5,5	0.30	0
5	ACT	B	505	-	1,3,3	0.83	0	0,3,3	0.00	-
4	GOL	A	504	-	5,5,5	0.80	0	5,5,5	0.71	0
4	GOL	C	504	-	5,5,5	0.21	0	5,5,5	0.70	0
3	2PG	C	503	2	7,10,10	1.45	1 (14%)	8,14,14	2.30	2 (25%)

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	2PG	A	503	2	-	0/7/11/11	-
6	PEG	C	507	-	-	2/4/4/4	-
3	2PG	D	503	2	-	0/7/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	508	-	-	3/4/4/4	-
3	2PG	B	503	2	-	0/7/11/11	-
6	PEG	D	505	-	-	3/4/4/4	-
4	GOL	A	504	-	-	4/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
3	2PG	C	503	2	-	0/7/11/11	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	2PG	P-O1P	2.94	1.64	1.59
3	D	503	2PG	O1P-C2	-2.55	1.42	1.45
5	C	506	ACT	CH3-C	2.54	1.52	1.48
5	D	504	ACT	CH3-C	2.43	1.51	1.48
5	C	505	ACT	CH3-C	2.40	1.51	1.48
5	B	504	ACT	CH3-C	2.24	1.51	1.48
5	A	505	ACT	CH3-C	2.11	1.51	1.48
3	A	503	2PG	C3-C2	2.03	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	2PG	P-O1P-C2	-6.01	109.26	123.04
3	D	503	2PG	O3P-P-O2P	3.14	122.98	110.68
3	A	503	2PG	O3-C3-C2	3.04	119.55	111.42
3	D	503	2PG	O3-C3-C2	2.21	117.32	111.42
3	C	503	2PG	O4P-P-O3P	2.12	115.76	107.64

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O1-C1-C2-C3
4	A	504	GOL	C1-C2-C3-O3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
4	C	508	GOL	C1-C2-C3-O3
6	D	505	PEG	O1-C1-C2-O2
4	C	508	GOL	O1-C1-C2-C3
4	A	504	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	504	GOL	O2-C2-C3-O3
4	C	508	GOL	O2-C2-C3-O3
6	C	507	PEG	O2-C3-C4-O4
6	D	505	PEG	C1-C2-O2-C3
6	D	505	PEG	C4-C3-O2-C2
6	C	507	PEG	C1-C2-O2-C3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	2PG	1	0
5	D	504	ACT	2	0
6	C	507	PEG	1	0
5	B	505	ACT	4	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	425/436 (97%)	0.36	29 (6%)	17 16	19, 33, 58, 72	0
1	B	424/436 (97%)	0.23	16 (3%)	40 39	17, 27, 47, 71	0
1	C	426/436 (97%)	-0.05	1 (0%)	95 94	13, 22, 35, 57	0
1	D	424/436 (97%)	0.07	8 (1%)	66 65	13, 24, 41, 54	0
All	All	1699/1744 (97%)	0.15	54 (3%)	47 46	13, 26, 48, 72	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	VAL	7.3
1	B	258	GLY	4.7
1	A	263	ALA	4.5
1	B	158	ALA	4.4
1	A	266	MET	4.1
1	B	259	THR	4.0
1	B	247	PHE	3.8
1	A	249	THR	3.8
1	A	260	THR	3.8
1	B	267	THR	3.6
1	B	252	THR	3.5
1	A	251	GLY	3.4
1	A	28	ILE	3.3
1	A	258	GLY	3.2
1	A	273	LEU	3.2
1	A	267	THR	3.1
1	A	256	PHE	3.1
1	A	213	GLY	3.1
1	A	253	GLY	3.0
1	A	211	VAL	3.0
1	B	256	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	253	GLY	2.9
1	D	31	THR	2.8
1	A	328	VAL	2.8
1	A	299	ALA	2.8
1	A	1	MET	2.8
1	A	71	LEU	2.7
1	A	262	THR	2.7
1	D	28	ILE	2.7
1	D	252	THR	2.7
1	A	212	ALA	2.6
1	A	425	ALA	2.6
1	A	292	ASP	2.6
1	A	252	THR	2.5
1	D	78	VAL	2.5
1	D	425	ALA	2.4
1	B	265	GLN	2.4
1	B	269	PHE	2.4
1	A	323	GLY	2.4
1	D	30	GLY	2.4
1	A	30	GLY	2.4
1	A	120	ALA	2.3
1	A	31	THR	2.3
1	B	210	ASP	2.3
1	B	300	SER	2.3
1	B	260	THR	2.2
1	C	425	ALA	2.2
1	D	126	GLU	2.2
1	A	298	THR	2.1
1	D	251	GLY	2.1
1	B	282	ILE	2.1
1	B	299	ALA	2.1
1	A	300	SER	2.0
1	A	270	TYR	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 ⓘ

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(Å <sup>2</sup> )	Q<0.9
4	GOL	C	504	6/6	0.69	0.28	61,64,67,70	0
6	PEG	C	507	7/7	0.86	0.14	61,62,65,69	0
5	ACT	B	504	4/4	0.88	0.17	54,55,59,61	0
4	GOL	A	504	6/6	0.88	0.15	37,45,48,49	0
6	PEG	D	505	7/7	0.88	0.16	49,50,54,54	0
5	ACT	A	505	4/4	0.89	0.16	44,46,53,54	0
5	ACT	B	505	4/4	0.89	0.22	37,44,45,53	0
5	ACT	C	505	4/4	0.90	0.12	54,55,56,58	0
4	GOL	C	508	6/6	0.93	0.14	29,38,45,58	0
5	ACT	C	506	4/4	0.95	0.14	35,37,39,40	0
5	ACT	D	504	4/4	0.95	0.14	36,36,39,41	0
2	MG	B	501	1/1	0.97	0.06	33,33,33,33	0
2	MG	A	501	1/1	0.98	0.07	39,39,39,39	0
2	MG	D	501	1/1	0.98	0.06	27,27,27,27	0
3	2PG	A	503	11/11	0.98	0.11	26,30,33,33	0
3	2PG	D	503	11/11	0.98	0.10	17,19,21,21	0
2	MG	A	502	1/1	0.98	0.06	35,35,35,35	0
2	MG	B	502	1/1	0.99	0.05	28,28,28,28	0
2	MG	C	501	1/1	0.99	0.06	25,25,25,25	0
3	2PG	B	503	11/11	0.99	0.08	25,28,33,34	0
3	2PG	C	503	11/11	0.99	0.10	15,17,19,20	0
7	CL	D	506	1/1	0.99	0.09	30,30,30,30	0
2	MG	C	502	1/1	1.00	0.06	20,20,20,20	0
2	MG	D	502	1/1	1.00	0.06	19,19,19,19	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.