



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:01 AM GMT

PDB ID : 2VK1  
Title : CRYSTAL STRUCTURE OF THE SACCHAROMYCES CEREVISIAE  
PYRUVATE DECARBOXYLASE VARIANT D28A IN COMPLEX WITH  
ITS SUBSTRATE  
Authors : Kutter, S.; Weik, M.; Weiss, M.S.; Konig, S.  
Deposited on : 2007-12-16  
Resolution : 1.71 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

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

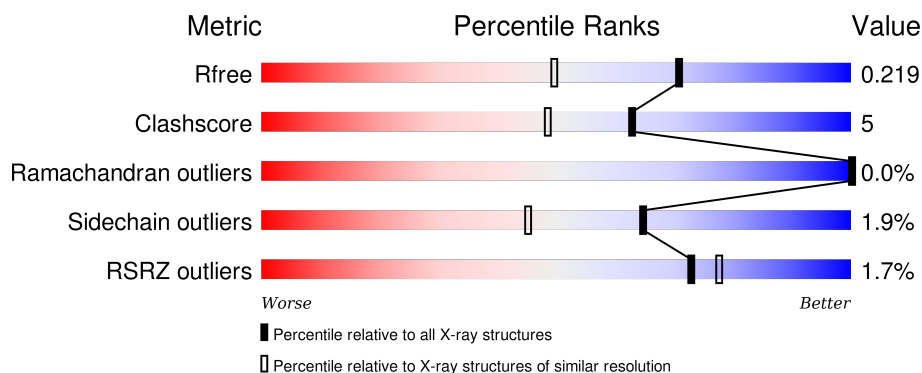
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.71 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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	563	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	B	563	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	C	563	<div> <div>2%</div> <div>91%</div> <div>9%</div> </div>
1	D	563	<div> <div>2%</div> <div>91%</div> <div>7%</div> </div>

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

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

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18994 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.

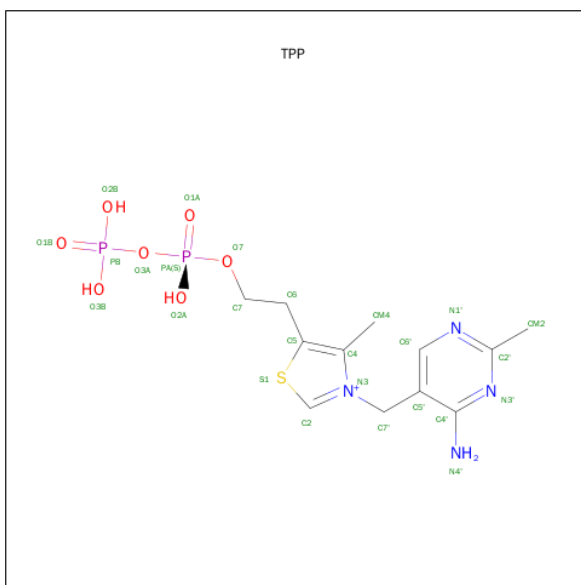
- Molecule 1 is a protein called PYRUVATE DECARBOXYLASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	0	0
			4320	2759	724	821	16			
1	B	562	Total	C	N	O	S	0	0	0
			4320	2759	724	821	16			
1	C	562	Total	C	N	O	S	0	0	0
			4320	2759	724	821	16			
1	D	562	Total	C	N	O	S	0	0	0
			4320	2759	724	821	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ALA	ASP	ENGINEERED MUTATION	UNP P06169
B	28	ALA	ASP	ENGINEERED MUTATION	UNP P06169
C	28	ALA	ASP	ENGINEERED MUTATION	UNP P06169
D	28	ALA	ASP	ENGINEERED MUTATION	UNP P06169

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).

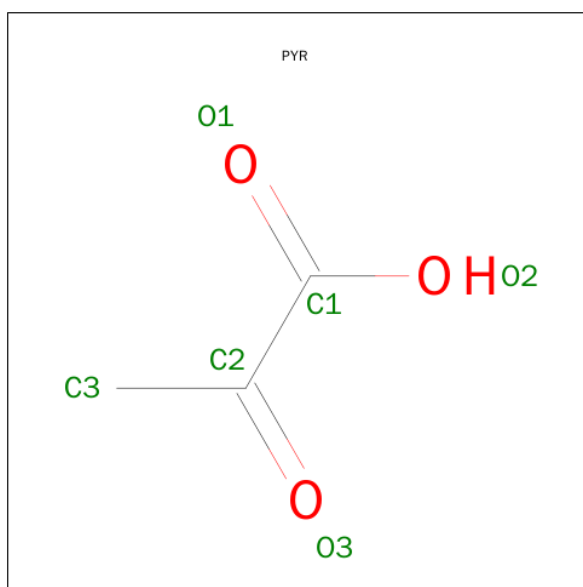


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- 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 PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).



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

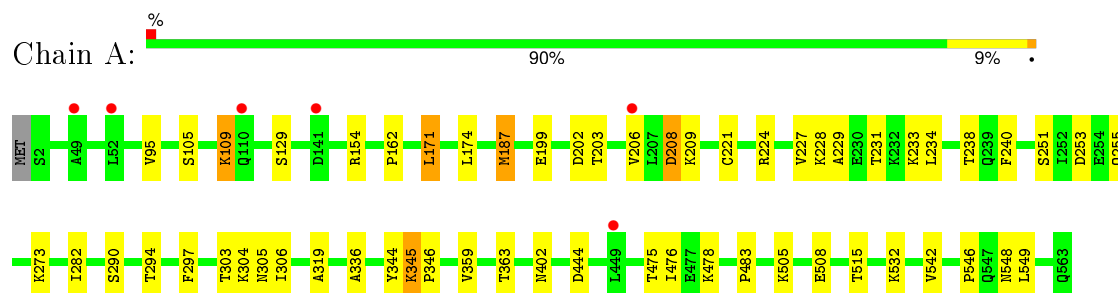
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	436	Total	O	0	0
			436	436		
5	B	377	Total	O	0	0
			377	377		
5	C	408	Total	O	0	0
			408	408		
5	D	337	Total	O	0	0
			337	337		

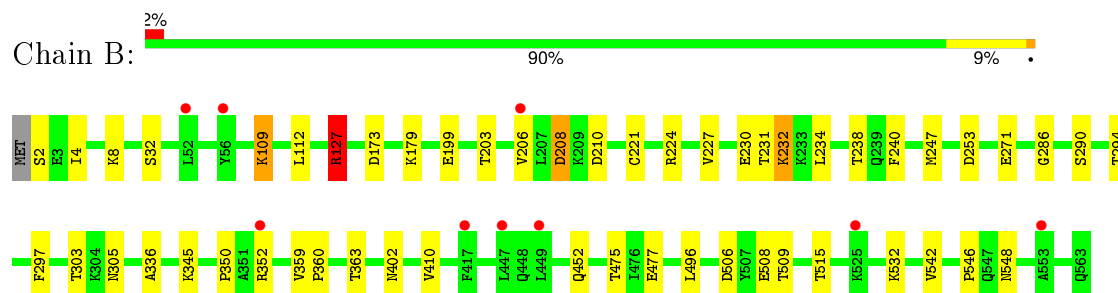
### 3 Residue-property plots [i](#)

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.

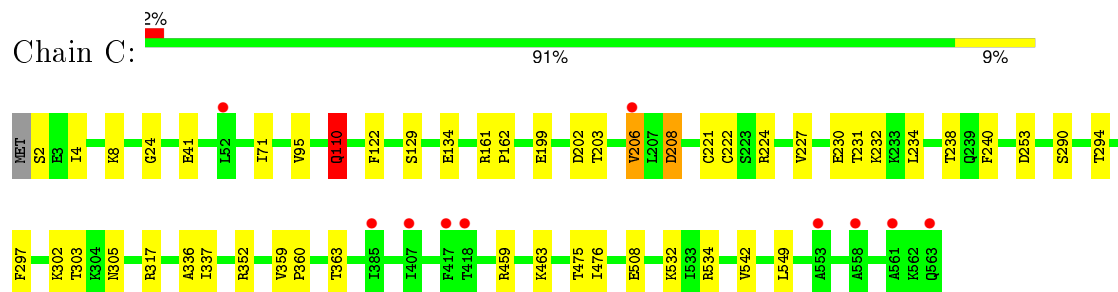
#### • Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1



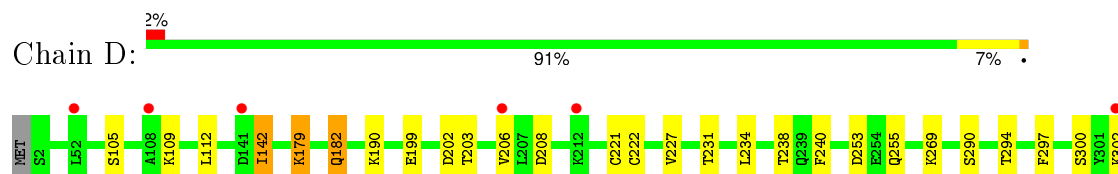
#### • Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1

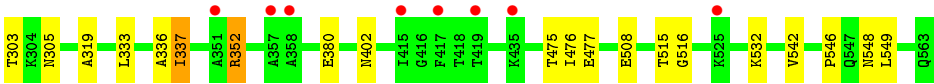


#### • Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1



#### • Molecule 1: PYRUVATE DECARBOXYLASE ISOZYME 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.88Å 141.31Å 114.41Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	109.11 – 1.71 39.46 – 1.71	Depositor EDS
% Data completeness (in resolution range)	99.1 (109.11-1.71) 99.1 (39.46-1.71)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.191 , 0.220 0.190 , 0.219	Depositor DCC
$R_{free}$ test set	1313 reflections (0.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 261646 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.77	1/4411 (0.0%)	0.71	1/5998 (0.0%)
1	B	0.81	5/4411 (0.1%)	0.73	2/5998 (0.0%)
1	C	0.76	3/4411 (0.1%)	0.70	1/5998 (0.0%)
1	D	0.70	0/4411	0.66	0/5998
All	All	0.76	9/17644 (0.1%)	0.70	4/23992 (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	7	0
1	B	8	0
1	C	8	0
1	D	8	0
All	All	31	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	208	ASP	CB-CG	-11.11	1.28	1.51
1	B	208	ASP	CB-CG	-8.89	1.33	1.51
1	B	232	LYS	CE-NZ	-7.92	1.29	1.49
1	B	230	GLU	CD-OE1	-6.33	1.18	1.25
1	A	208	ASP	CB-CG	-6.24	1.38	1.51
1	B	109	LYS	CB-CG	-5.86	1.36	1.52
1	C	208	ASP	CA-CB	-5.17	1.42	1.53
1	C	230	GLU	CD-OE1	-5.08	1.20	1.25
1	B	127	ARG	CB-CG	-5.06	1.38	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	ASP	CB-CG-OD1	-8.30	110.83	118.30
1	B	208	ASP	CB-CG-OD1	-7.19	111.83	118.30
1	A	444	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	208	ASP	OD1-CG-OD2	5.25	133.28	123.30

All (31) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	203	THR	CB
1	A	231	THR	CB
1	A	238	THR	CB
1	A	294	THR	CB
1	A	303	THR	CB
1	A	475	THR	CB
1	A	515	THR	CB
1	B	203	THR	CB
1	B	231	THR	CB
1	B	238	THR	CB
1	B	294	THR	CB
1	B	303	THR	CB
1	B	363	THR	CB
1	B	475	THR	CB
1	B	515	THR	CB
1	C	203	THR	CB
1	C	231	THR	CB
1	C	238	THR	CB
1	C	294	THR	CB
1	C	303	THR	CB
1	C	363	THR	CB
1	C	475	THR	CB
1	C	515	THR	CB
1	D	203	THR	CB
1	D	231	THR	CB
1	D	238	THR	CB
1	D	294	THR	CB
1	D	303	THR	CB
1	D	363	THR	CB
1	D	475	THR	CB
1	D	515	THR	CB

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	4320	0	4329	54	0
1	B	4320	0	4330	41	0
1	C	4320	0	4330	42	0
1	D	4320	0	4330	45	0
2	A	26	0	15	0	0
2	B	26	0	15	1	0
2	C	26	0	15	1	0
2	D	26	0	15	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	12	0	6	4	0
4	B	12	0	6	5	0
4	C	12	0	6	6	0
4	D	12	0	6	4	0
5	A	436	0	0	10	0
5	B	377	0	0	9	0
5	C	408	0	0	6	0
5	D	337	0	0	6	0
All	All	18994	0	17403	183	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 (183) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:CYS:SG	4:C:603:PYP:C2	2.14	1.35
1:B:221:CYS:SG	4:B:603:PYP:C2	2.18	1.32
1:C:336:ALA:HB2	5:C:2239:HOH:O	1.43	1.15
1:B:336:ALA:HB2	5:B:2245:HOH:O	1.45	1.14
1:D:303:THR:HG22	1:D:305:ASN:H	1.19	1.08
1:C:303:THR:HG22	1:C:305:ASN:H	1.17	1.07
1:D:294:THR:HG23	1:D:297:PHE:H	1.18	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:294:THR:HG23	1:C:297:PHE:H	1.23	1.01
1:B:303:THR:HG22	1:B:305:ASN:H	1.25	1.01
1:D:336:ALA:HB2	5:D:2194:HOH:O	1.60	1.01
1:B:294:THR:HG23	1:B:297:PHE:H	1.22	1.01
1:A:238:THR:HG23	1:A:240:PHE:H	1.23	1.01
1:C:238:THR:HG23	1:C:240:PHE:H	1.28	0.98
1:A:336:ALA:HB2	5:A:2252:HOH:O	1.63	0.96
1:A:303:THR:HG22	1:A:305:ASN:H	1.29	0.96
1:A:187:MET:HA	1:A:187:MET:CE	1.96	0.95
1:A:294:THR:HG23	1:A:297:PHE:H	1.33	0.94
1:B:238:THR:HG23	1:B:240:PHE:H	1.34	0.93
1:C:336:ALA:HB2	5:C:2240:HOH:O	1.69	0.91
1:A:187:MET:HA	1:A:187:MET:HE3	1.52	0.91
1:A:206:VAL:CG2	5:A:2155:HOH:O	2.17	0.90
5:B:2052:HOH:O	1:C:317:ARG:HD2	1.72	0.87
1:B:203:THR:HG21	5:B:2153:HOH:O	1.75	0.87
1:D:227:VAL:O	1:D:231:THR:HG23	1.75	0.86
1:A:221:CYS:SG	4:A:603:PYR:C3	2.64	0.86
1:A:154:ARG:HA	1:A:187:MET:HE1	1.58	0.85
1:D:203:THR:HG21	5:D:2122:HOH:O	1.76	0.85
1:C:221:CYS:SG	4:C:603:PYR:C3	2.67	0.83
1:A:203:THR:HG21	5:A:2151:HOH:O	1.79	0.83
1:D:238:THR:HG23	1:D:240:PHE:H	1.45	0.81
1:A:290:SER:O	1:A:294:THR:HG22	1.79	0.81
1:C:203:THR:HG21	5:C:2151:HOH:O	1.80	0.81
1:B:227:VAL:O	1:B:231:THR:HG23	1.81	0.81
1:C:360:PRO:O	1:C:363:THR:HG23	1.83	0.79
1:C:290:SER:O	1:C:294:THR:HG22	1.83	0.79
1:B:234:LEU:O	1:B:238:THR:HG22	1.84	0.78
1:B:290:SER:O	1:B:294:THR:HG22	1.83	0.77
1:D:234:LEU:O	1:D:238:THR:HG22	1.85	0.76
1:D:352:ARG:HH11	1:D:352:ARG:HG2	1.47	0.75
1:B:221:CYS:SG	4:B:603:PYR:C3	2.74	0.75
1:C:303:THR:HG22	1:C:305:ASN:N	1.99	0.74
1:B:206:VAL:HG13	5:B:2158:HOH:O	1.86	0.74
1:A:227:VAL:O	1:A:231:THR:HG23	1.88	0.74
1:A:303:THR:HG23	5:A:2228:HOH:O	1.87	0.73
1:A:199:GLU:O	1:A:203:THR:HG23	1.88	0.73
1:D:179:LYS:HE3	1:D:182:GLN:HG3	1.70	0.72
1:D:290:SER:O	1:D:294:THR:HG22	1.89	0.72
1:D:221:CYS:SG	4:D:603:PYR:C1	2.76	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:VAL:HB	1:C:363:THR:HG21	1.74	0.70
1:B:199:GLU:O	1:B:203:THR:HG23	1.90	0.70
1:D:199:GLU:O	1:D:203:THR:HG23	1.92	0.70
1:B:360:PRO:O	1:B:363:THR:HG23	1.93	0.69
1:D:221:CYS:SG	4:D:603:PYR:C3	2.80	0.69
1:D:294:THR:CG2	1:D:297:PHE:H	2.02	0.69
1:B:221:CYS:SG	4:B:603:PYR:C1	2.81	0.68
1:A:221:CYS:SG	4:A:603:PYR:C1	2.80	0.68
1:C:234:LEU:O	1:C:238:THR:HG22	1.94	0.67
1:C:221:CYS:SG	4:C:603:PYR:C1	2.82	0.67
1:C:294:THR:CG2	1:C:297:PHE:H	2.03	0.67
1:B:127:ARG:HG2	1:B:127:ARG:HH11	1.59	0.66
1:A:187:MET:HE2	1:A:187:MET:HA	1.75	0.66
1:A:203:THR:O	1:A:206:VAL:HG22	1.96	0.65
1:C:227:VAL:O	1:C:231:THR:HG23	1.96	0.65
1:B:508:GLU:HG3	1:B:532:LYS:HD2	1.79	0.65
1:B:294:THR:HG23	1:B:297:PHE:N	2.05	0.65
1:D:303:THR:HG22	1:D:305:ASN:N	2.02	0.65
1:D:475:THR:HG22	1:D:542:VAL:O	1.98	0.64
1:B:206:VAL:HG11	5:B:2055:HOH:O	1.98	0.63
2:C:600:TPP:H7'2	4:C:602:PYR:C1	2.29	0.62
1:A:221:CYS:CB	4:A:603:PYR:C2	2.78	0.62
1:D:300:SER:O	1:D:302:LYS:HE2	1.99	0.62
1:D:203:THR:O	1:D:206:VAL:HG12	1.98	0.62
1:B:359:VAL:HB	1:B:363:THR:HG21	1.81	0.61
1:D:380:GLU:HG2	1:D:402:ASN:O	2.00	0.61
1:A:336:ALA:CB	5:A:2252:HOH:O	2.35	0.61
1:B:206:VAL:HG23	5:B:2059:HOH:O	2.02	0.59
1:D:105:SER:O	1:D:109:LYS:HG2	2.01	0.59
1:D:206:VAL:HG13	5:D:2125:HOH:O	2.03	0.59
1:D:179:LYS:CE	1:D:182:GLN:HG3	2.32	0.59
1:A:234:LEU:O	1:A:238:THR:HG22	2.03	0.59
1:A:508:GLU:HG3	1:A:532:LYS:HD2	1.84	0.59
1:C:202:ASP:O	1:C:206:VAL:CG1	2.51	0.58
1:A:154:ARG:HA	1:A:187:MET:CE	2.32	0.58
1:D:206:VAL:CG1	5:D:2125:HOH:O	2.51	0.58
1:C:202:ASP:O	1:C:206:VAL:HG12	2.04	0.58
1:A:206:VAL:HG21	5:A:2155:HOH:O	1.92	0.57
1:D:182:GLN:HE21	1:D:182:GLN:HA	1.70	0.57
1:A:202:ASP:O	1:A:206:VAL:HG13	2.03	0.57
1:B:127:ARG:CG	1:B:127:ARG:HH11	2.18	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:GLU:O	1:C:203:THR:HG23	2.06	0.55
1:A:363:THR:HB	1:A:515:THR:CG2	2.35	0.55
1:A:475:THR:HG22	1:A:542:VAL:O	2.07	0.55
1:D:352:ARG:NH1	1:D:352:ARG:HG2	2.19	0.55
1:D:294:THR:HG23	1:D:297:PHE:N	2.03	0.54
1:D:333:LEU:O	1:D:337:ILE:HB	2.08	0.54
1:B:232:LYS:HE3	5:B:2171:HOH:O	2.06	0.53
1:C:459:ARG:NH1	5:C:2326:HOH:O	2.38	0.53
1:A:359:VAL:HG23	1:A:515:THR:HG21	1.91	0.53
1:C:475:THR:HG22	1:C:542:VAL:O	2.09	0.52
1:A:171:LEU:HD12	1:A:174:LEU:HD12	1.90	0.52
1:D:476:ILE:HG13	1:D:549:LEU:HD11	1.91	0.52
1:D:221:CYS:CB	4:D:603:PYR:C2	2.88	0.52
1:A:206:VAL:HG23	5:A:2155:HOH:O	1.97	0.52
1:A:363:THR:HB	1:A:515:THR:HG22	1.93	0.51
1:B:294:THR:CG2	1:B:297:PHE:H	2.11	0.51
1:C:221:CYS:CB	4:C:603:PYR:C2	2.89	0.51
1:C:206:VAL:HG22	5:C:2155:HOH:O	2.11	0.51
1:A:303:THR:HG22	1:A:305:ASN:N	2.12	0.50
1:B:206:VAL:CG1	5:B:2158:HOH:O	2.52	0.50
1:A:187:MET:CE	1:A:187:MET:CA	2.75	0.49
1:A:228:LYS:HE3	1:A:251:SER:HA	1.94	0.49
1:B:477:GLU:OE2	4:B:602:PYR:O2	2.31	0.49
1:B:475:THR:HG22	1:B:542:VAL:O	2.11	0.49
1:A:105:SER:O	1:A:109:LYS:HG3	2.12	0.49
1:C:134:GLU:HB2	1:C:161:ARG:HB2	1.94	0.49
1:D:546:PRO:HB2	1:D:548:ASN:OD1	2.13	0.48
1:C:303:THR:HG21	1:C:305:ASN:HB3	1.96	0.48
1:C:95:VAL:O	1:C:162:PRO:HA	2.14	0.48
1:D:255:GLN:HB2	1:D:402:ASN:OD1	2.13	0.48
1:A:95:VAL:O	1:A:162:PRO:HA	2.13	0.47
1:B:224:ARG:HA	1:B:224:ARG:CZ	2.44	0.47
1:C:221:CYS:SG	4:C:603:PYR:H32	2.51	0.47
1:A:515:THR:HG23	5:A:2283:HOH:O	2.13	0.47
1:D:206:VAL:HG23	5:D:2129:HOH:O	2.14	0.47
1:A:303:THR:HG22	1:A:304:LYS:N	2.30	0.46
1:B:247:MET:HE2	1:B:410:VAL:HB	1.95	0.46
2:B:600:TPP:H7'2	4:B:602:PYR:C1	2.45	0.46
1:A:187:MET:HE2	1:A:187:MET:CA	2.40	0.46
1:A:294:THR:CG2	1:A:297:PHE:H	2.15	0.46
1:C:232:LYS:NZ	1:C:253:ASP:OD2	2.48	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:HE2	5:A:2206:HOH:O	2.15	0.46
1:C:508:GLU:HG3	1:C:532:LYS:HD2	1.97	0.46
1:A:253:ASP:HB3	1:A:402:ASN:OD1	2.16	0.45
1:A:476:ILE:HG13	1:A:549:LEU:HD11	1.99	0.45
1:D:475:THR:CG2	1:D:542:VAL:O	2.63	0.45
1:C:336:ALA:CB	5:C:2239:HOH:O	2.26	0.45
1:B:127:ARG:CG	1:B:127:ARG:NH1	2.80	0.45
1:D:508:GLU:HG3	1:D:532:LYS:HD2	1.99	0.44
1:C:549:LEU:O	1:C:549:LEU:HD12	2.18	0.44
1:D:477:GLU:OE2	4:D:602:PYR:O2	2.36	0.44
1:D:179:LYS:NZ	1:D:182:GLN:HG3	2.32	0.44
1:B:303:THR:HG22	1:B:305:ASN:N	2.10	0.44
1:D:222:CYS:SG	1:D:231:THR:HG21	2.57	0.44
1:C:476:ILE:HG13	1:C:549:LEU:HD11	1.99	0.43
1:C:4:ILE:HG12	1:C:8:LYS:HB3	2.00	0.43
1:B:271:GLU:HB3	1:B:350:PRO:HB3	1.99	0.43
1:B:336:ALA:CB	5:B:2245:HOH:O	2.28	0.43
1:B:253:ASP:HB3	1:B:402:ASN:OD1	2.18	0.43
1:A:546:PRO:HB2	1:A:548:ASN:OD1	2.19	0.43
1:C:303:THR:CG2	1:C:305:ASN:HB3	2.49	0.43
1:C:24:GLY:HA3	1:C:71:ILE:O	2.19	0.43
1:D:253:ASP:HB3	1:D:402:ASN:OD1	2.20	0.42
1:A:229:ALA:O	1:A:233:LYS:HG3	2.19	0.42
1:A:221:CYS:SG	4:A:603:PYR:H32	2.58	0.42
1:D:269:LYS:HB3	1:D:269:LYS:HE2	1.83	0.42
1:D:190:LYS:HB2	1:D:190:LYS:HE3	1.86	0.42
1:B:4:ILE:HG12	1:B:8:LYS:HB3	2.02	0.42
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.55	0.42
1:B:32:SER:OG	1:B:173:ASP:OD2	2.32	0.42
1:A:224:ARG:CZ	1:A:224:ARG:HA	2.50	0.42
1:A:345:LYS:H	1:A:345:LYS:HG2	1.68	0.42
1:B:221:CYS:HB2	1:B:286:GLY:CA	2.51	0.41
1:C:532:LYS:HE3	1:C:532:LYS:HB3	1.82	0.41
1:C:110:GLN:HB3	1:C:122:PHE:HE2	1.85	0.41
1:A:224:ARG:HD2	5:A:2166:HOH:O	2.18	0.41
1:A:319:ALA:HB1	1:D:319:ALA:HB1	2.01	0.41
1:D:202:ASP:HB2	5:D:2124:HOH:O	2.20	0.41
1:D:179:LYS:HA	1:D:179:LYS:HD2	1.58	0.41
1:A:282:ILE:HD12	1:A:306:ILE:HD12	2.03	0.41
1:B:363:THR:HB	1:B:515:THR:HG22	2.02	0.41
1:C:222:CYS:SG	1:C:231:THR:HG21	2.61	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:508:GLU:HB2	1:C:534:ARG:HG2	2.03	0.41
1:D:142:ILE:HG13	1:D:142:ILE:H	1.53	0.41
1:C:303:THR:CG2	1:C:305:ASN:CB	2.99	0.40
1:B:203:THR:O	1:B:206:VAL:HG12	2.21	0.40
1:A:475:THR:CG2	1:A:542:VAL:O	2.69	0.40
1:A:478:LYS:HB3	1:A:483:PRO:HA	2.03	0.40
1:C:224:ARG:CZ	1:C:224:ARG:HA	2.51	0.40
1:A:255:GLN:HB2	1:A:402:ASN:OD1	2.20	0.40
1:B:496:LEU:HD22	1:B:509:THR:HB	2.03	0.40
1:B:506:ASP:OD1	1:B:532:LYS:HE3	2.21	0.40
1:B:546:PRO:HB2	1:B:548:ASN:OD1	2.21	0.40
1:D:515:THR:HG23	1:D:516:GLY:N	2.35	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	560/563 (100%)	551 (98%)	9 (2%)	0	100	100
1	B	560/563 (100%)	546 (98%)	14 (2%)	0	100	100
1	C	560/563 (100%)	546 (98%)	13 (2%)	1 (0%)	52	32
1	D	560/563 (100%)	550 (98%)	10 (2%)	0	100	100
All	All	2240/2252 (100%)	2193 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	110	GLN

### 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	465/466 (100%)	457 (98%)	8 (2%)	68	50
1	B	465/466 (100%)	455 (98%)	10 (2%)	60	38
1	C	465/466 (100%)	455 (98%)	10 (2%)	60	38
1	D	465/466 (100%)	458 (98%)	7 (2%)	72	55
All	All	1860/1864 (100%)	1825 (98%)	35 (2%)	65	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	LYS
1	A	129	SER
1	A	171	LEU
1	A	187	MET
1	A	208	ASP
1	A	209	LYS
1	A	345	LYS
1	A	505	LYS
1	B	2	SER
1	B	109	LYS
1	B	112	LEU
1	B	127	ARG
1	B	179	LYS
1	B	208	ASP
1	B	210	ASP
1	B	345	LYS
1	B	352	ARG
1	B	452	GLN
1	C	2	SER
1	C	41	GLU
1	C	110	GLN
1	C	129	SER
1	C	206	VAL
1	C	208	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	302	LYS
1	C	337	ILE
1	C	352	ARG
1	C	463	LYS
1	D	112	LEU
1	D	142	ILE
1	D	179	LYS
1	D	182	GLN
1	D	208	ASP
1	D	337	ILE
1	D	352	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	486	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
2	TPP	A	600	3,4	20,27,27	1.51	3 (15%)	31,40,40	1.32	4 (12%)
4	PYR	A	602	2	2,5,5	0.98	0	2,6,6	6.79	2 (100%)
4	PYR	A	603	1	2,5,5	1.05	0	2,6,6	2.72	1 (50%)
2	TPP	B	600	3,4	20,27,27	1.01	1 (5%)	31,40,40	1.43	3 (9%)
4	PYR	B	602	2	2,5,5	0.75	0	2,6,6	5.65	2 (100%)
4	PYR	B	603	-	2,5,5	1.23	0	2,6,6	1.32	0
2	TPP	C	600	3,4	20,27,27	1.70	5 (25%)	31,40,40	1.45	5 (16%)
4	PYR	C	602	2	2,5,5	0.83	0	2,6,6	6.66	2 (100%)
4	PYR	C	603	-	2,5,5	1.50	0	2,6,6	2.45	1 (50%)
2	TPP	D	600	3,4	20,27,27	1.47	5 (25%)	31,40,40	1.47	5 (16%)
4	PYR	D	602	2	2,5,5	0.85	0	2,6,6	4.28	2 (100%)
4	PYR	D	603	1	2,5,5	1.32	0	2,6,6	3.14	2 (100%)

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
2	TPP	A	600	3,4	-	0/16/17/17	0/2/2/2
4	PYR	A	602	2	-	0/0/4/4	0/0/0/0
4	PYR	A	603	1	-	0/0/4/4	0/0/0/0
2	TPP	B	600	3,4	-	0/16/17/17	0/2/2/2
4	PYR	B	602	2	-	0/0/4/4	0/0/0/0
4	PYR	B	603	-	-	0/0/4/4	0/0/0/0
2	TPP	C	600	3,4	-	0/16/17/17	0/2/2/2
4	PYR	C	602	2	-	0/0/4/4	0/0/0/0
4	PYR	C	603	-	-	0/0/4/4	0/0/0/0
2	TPP	D	600	3,4	-	0/16/17/17	0/2/2/2
4	PYR	D	602	2	-	0/0/4/4	0/0/0/0
4	PYR	D	603	1	-	0/0/4/4	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	TPP	C4-N3	-4.94	1.35	1.39
2	A	600	TPP	C4-N3	-3.74	1.36	1.39
2	D	600	TPP	C4-N3	-2.85	1.37	1.39
2	C	600	TPP	C2'-N3'	2.02	1.37	1.34
2	B	600	TPP	C6'-N1'	2.15	1.39	1.34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	TPP	C2'-N1'	2.25	1.38	1.34
2	D	600	TPP	C2'-N1'	2.33	1.38	1.34
2	D	600	TPP	C2'-N3'	2.48	1.38	1.34
2	D	600	TPP	C6'-N1'	2.50	1.39	1.34
2	C	600	TPP	C4'-N3'	2.57	1.39	1.35
2	C	600	TPP	C6'-N1'	2.66	1.40	1.34
2	A	600	TPP	C6'-N1'	2.67	1.40	1.34
2	D	600	TPP	C4'-N3'	2.76	1.39	1.35
2	A	600	TPP	C2'-N1'	3.25	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	602	PYR	O3-C2-C3	-8.35	100.12	120.13
4	A	602	PYR	O3-C2-C3	-7.30	102.64	120.13
4	B	602	PYR	O3-C2-C3	-7.04	103.25	120.13
4	A	602	PYR	C3-C2-C1	-6.25	101.65	120.23
4	D	602	PYR	O3-C2-C3	-4.94	108.30	120.13
4	C	602	PYR	C3-C2-C1	-4.36	107.25	120.23
2	C	600	TPP	N1'-C2'-N3'	-3.85	118.47	125.60
4	B	602	PYR	C3-C2-C1	-3.79	108.96	120.23
2	B	600	TPP	N1'-C2'-N3'	-3.76	118.65	125.60
2	A	600	TPP	N1'-C2'-N3'	-3.62	118.89	125.60
4	D	602	PYR	C3-C2-C1	-3.51	109.80	120.23
4	A	603	PYR	O3-C2-C3	-3.40	111.98	120.13
4	D	603	PYR	C3-C2-C1	-3.34	110.30	120.23
4	C	603	PYR	O3-C2-C3	-3.30	112.23	120.13
2	D	600	TPP	N1'-C2'-N3'	-3.15	119.77	125.60
4	D	603	PYR	O3-C2-C3	-2.93	113.12	120.13
2	D	600	TPP	C5'-C6'-N1'	-2.27	119.92	123.86
2	C	600	TPP	C2'-N3'-C4'	2.01	122.19	118.19
2	D	600	TPP	O3A-PA-O7	2.14	108.61	102.94
2	A	600	TPP	C2'-N3'-C4'	2.19	122.54	118.19
2	A	600	TPP	C6'-N1'-C2'	2.25	119.71	115.77
2	C	600	TPP	CM2-C2'-N1'	2.40	119.91	117.03
2	C	600	TPP	CM2-C2'-N3'	2.59	121.61	117.20
2	C	600	TPP	C6'-N1'-C2'	2.76	120.59	115.77
2	D	600	TPP	C6'-N1'-C2'	3.07	121.13	115.77
2	B	600	TPP	C6'-N1'-C2'	3.23	121.42	115.77
2	A	600	TPP	CM2-C2'-N1'	3.47	121.20	117.03
2	B	600	TPP	CM2-C2'-N1'	3.50	121.23	117.03
2	D	600	TPP	CM2-C2'-N1'	4.20	122.07	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	PYR	4	0
2	B	600	TPP	1	0
4	B	602	PYR	2	0
4	B	603	PYR	3	0
2	C	600	TPP	1	0
4	C	602	PYR	1	0
4	C	603	PYR	5	0
4	D	602	PYR	1	0
4	D	603	PYR	3	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	562/563 (99%)	-0.19	6 (1%) 82 86	10, 18, 30, 39	0
1	B	562/563 (99%)	-0.18	9 (1%) 74 79	10, 17, 27, 38	0
1	C	562/563 (99%)	-0.13	10 (1%) 71 76	11, 19, 31, 41	0
1	D	562/563 (99%)	-0.01	14 (2%) 61 65	12, 22, 35, 40	0
All	All	2248/2252 (99%)	-0.13	39 (1%) 73 77	10, 19, 32, 41	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	561	ALA	3.9
1	D	358	ALA	3.5
1	D	206	VAL	3.1
1	D	351	ALA	3.0
1	D	212	LYS	3.0
1	D	108	ALA	2.9
1	C	558	ALA	2.9
1	C	563	GLN	2.8
1	C	206	VAL	2.8
1	D	357	ALA	2.8
1	B	352	ARG	2.6
1	B	553	ALA	2.5
1	B	52	LEU	2.5
1	D	52	LEU	2.5
1	C	407	ILE	2.4
1	B	449	LEU	2.4
1	C	52	LEU	2.4
1	A	206	VAL	2.4
1	C	417	PHE	2.3
1	C	553	ALA	2.3
1	A	110	GLN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	2.3
1	B	525	LYS	2.3
1	A	52	LEU	2.3
1	A	49	ALA	2.3
1	A	141	ASP	2.2
1	B	447	LEU	2.2
1	D	302	LYS	2.2
1	C	385	ILE	2.2
1	B	417	PHE	2.1
1	D	435	LYS	2.1
1	C	418	THR	2.1
1	D	141	ASP	2.1
1	D	525	LYS	2.1
1	B	56	TYR	2.1
1	A	449	LEU	2.1
1	D	415	ILE	2.0
1	D	417	PHE	2.0
1	D	419	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
4	PYR	C	603	6/6	0.86	0.10	2.98	23,23,25,25	0
4	PYR	B	603	6/6	0.94	0.07	1.46	16,19,20,21	0
4	PYR	C	602	6/6	0.85	0.11	1.30	34,38,39,39	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PYR	A	602	6/6	0.88	0.11	1.06	32,34,35,36	0
4	PYR	D	603	6/6	0.96	0.08	0.85	24,26,27,28	0
4	PYR	A	603	6/6	0.94	0.07	0.65	22,23,25,26	0
4	PYR	B	602	6/6	0.85	0.11	0.48	32,33,35,35	0
4	PYR	D	602	6/6	0.89	0.10	0.36	33,35,37,39	0
3	MG	D	601	1/1	0.99	0.08	0.25	19,19,19,19	0
3	MG	A	601	1/1	0.99	0.08	0.09	15,15,15,15	0
2	TPP	A	600	26/26	0.98	0.09	-0.29	10,13,15,15	0
2	TPP	C	600	26/26	0.98	0.09	-0.46	13,15,18,20	0
2	TPP	B	600	26/26	0.98	0.09	-0.54	10,13,15,16	0
3	MG	C	601	1/1	0.98	0.07	-0.55	17,17,17,17	0
2	TPP	D	600	26/26	0.98	0.07	-0.81	13,15,16,17	0
3	MG	B	601	1/1	0.98	0.05	-1.80	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.