



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:24 PM GMT

PDB ID : 4RJJ  
Title : Acetolactate synthase from Bacillus subtilis bound to ThDP - crystal form II  
Authors : Sommer, B.; von Moeller, H.; Haack, M.; Qoura, F.; Langner, C.; Bourenkov, G.; Garbe, D.; Brueck, T.; Loll, B.  
Deposited on : 2014-10-09  
Resolution : 2.34 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

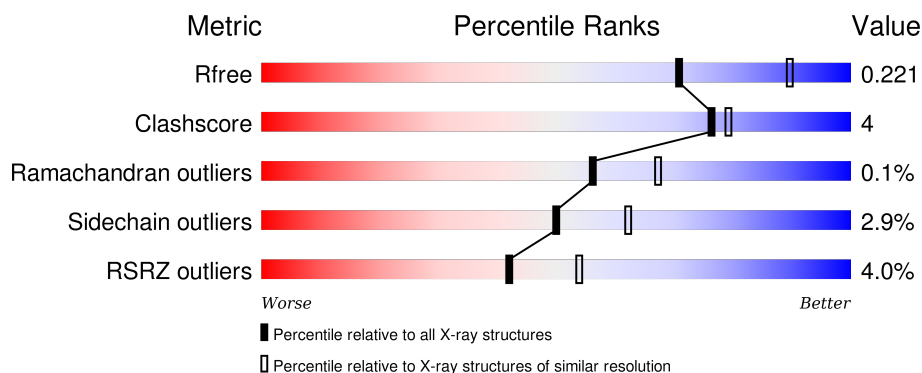
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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	571	<div> <div>4%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
1	B	571	<div> <div>5%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
1	C	571	<div> <div>4%</div> <div>88%</div> <div>8%</div> <div>• •</div> </div>
1	D	571	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
1	E	571	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	571	
1	G	571	
1	H	571	

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	PG4	A	605	-	-	-	X
4	PG4	B	605	-	-	-	X
4	PG4	B	606	-	-	-	X
4	PG4	C	606	-	-	-	X
4	PG4	D	603	-	-	-	X
4	PG4	E	603	-	-	X	X
4	PG4	E	605	-	-	-	X
4	PG4	E	606	-	-	-	X
4	PG4	E	607	-	-	-	X
4	PG4	F	603	-	-	-	X
4	PG4	G	604	-	-	-	X
4	PG4	G	606	-	-	-	X
4	PG4	H	605	-	-	-	X
5	ACT	D	608	-	-	-	X

## 2 Entry composition

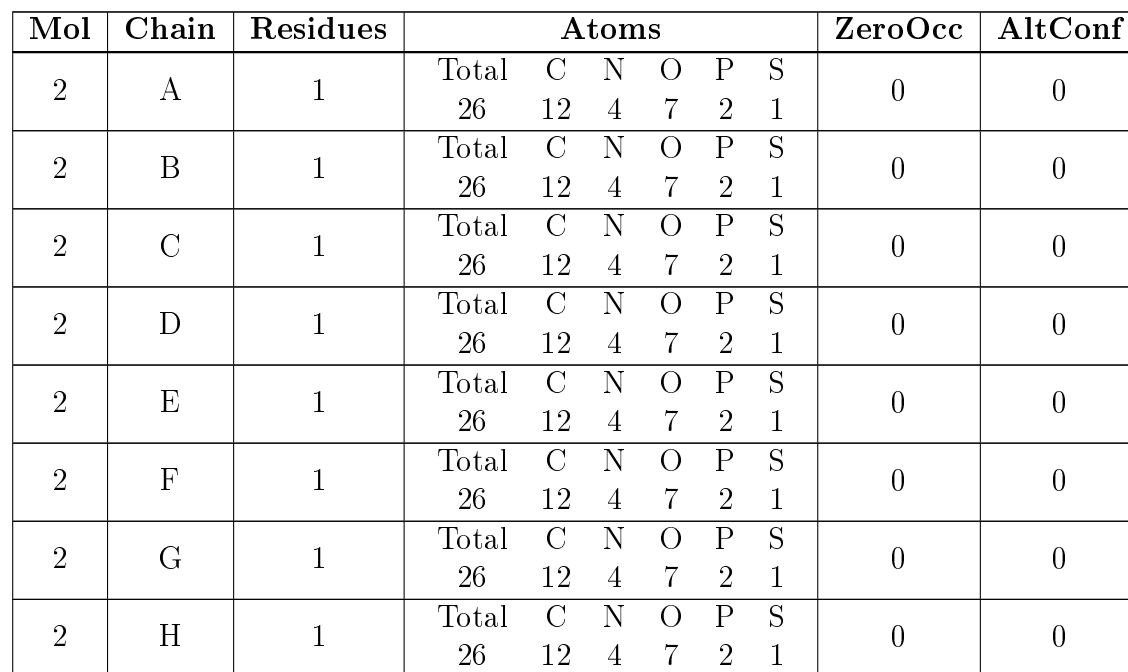
There are 6 unique types of molecules in this entry. The entry contains 36626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Acetolactate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	2	0
			4261	2704	732	813	12			
1	B	553	Total	C	N	O	S	0	3	0
			4250	2697	729	812	12			
1	C	553	Total	C	N	O	S	0	5	0
			4259	2702	730	814	13			
1	D	553	Total	C	N	O	S	0	9	0
			4276	2723	729	812	12			
1	E	555	Total	C	N	O	S	0	5	0
			4281	2722	734	813	12			
1	F	553	Total	C	N	O	S	0	1	0
			4241	2692	728	809	12			
1	G	554	Total	C	N	O	S	0	1	0
			4250	2696	730	812	12			
1	H	553	Total	C	N	O	S	0	2	0
			4248	2695	729	812	12			

- 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).



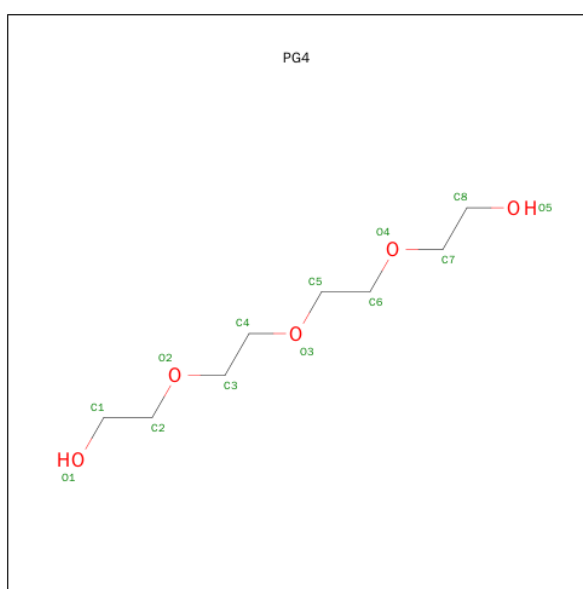
- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | G     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | D     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | E     | 1        | Total Mg<br>1 1 | 0       | 0       |
| 3   | H     | 1        | Total Mg<br>1 1 | 0       | 0       |



*Continued from previous page...*

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

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			13	8	5		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		

*Continued on next page...*

*Continued from previous page...*

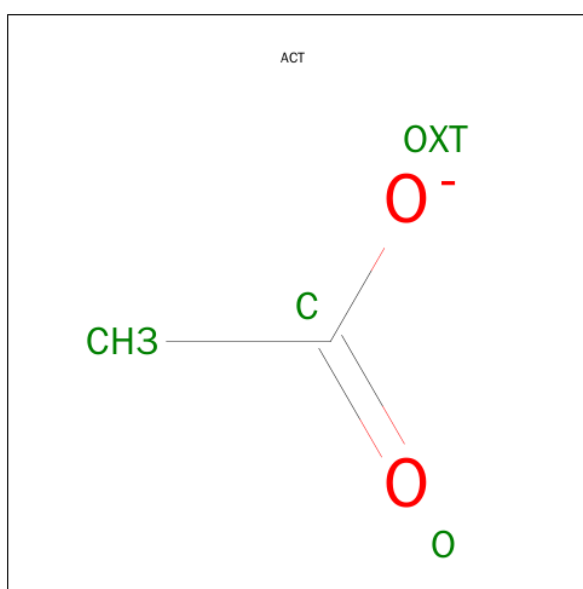
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			13	8	5		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			13	8	5		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	E	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			13	8	5		
4	F	1	Total	C	O	0	0
			10	6	4		
4	G	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			11	7	4		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			8	5	3		
4	H	1	Total	C	O	0	0
			13	8	5		
4	H	1	Total	C	O	0	0
			10	6	4		
4	H	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	215	Total	O	0	0
			215	215		
6	B	259	Total	O	0	2
			259	259		
6	C	277	Total	O	0	2
			277	277		
6	D	245	Total	O	0	0
			245	245		

*Continued on next page...*



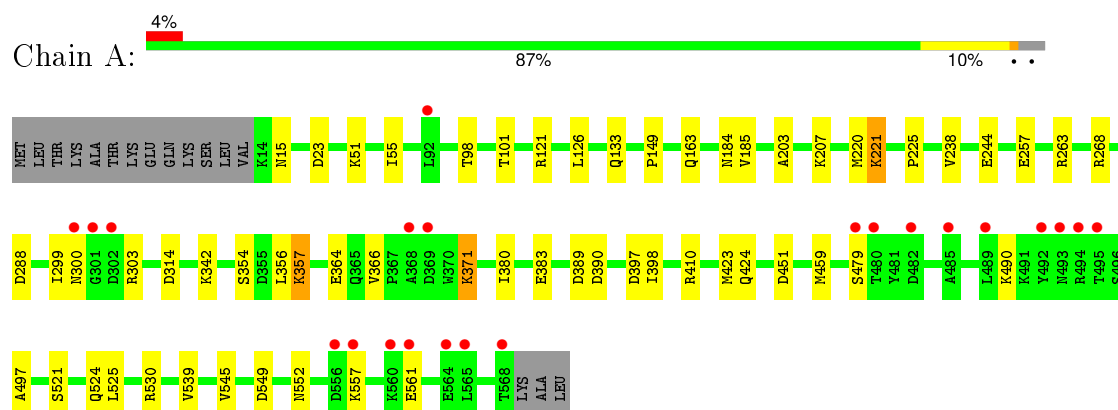
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	260	Total 260	O 260	0	1
6	F	264	Total 264	O 264	0	0
6	G	232	Total 232	O 232	0	0
6	H	203	Total 203	O 203	0	2

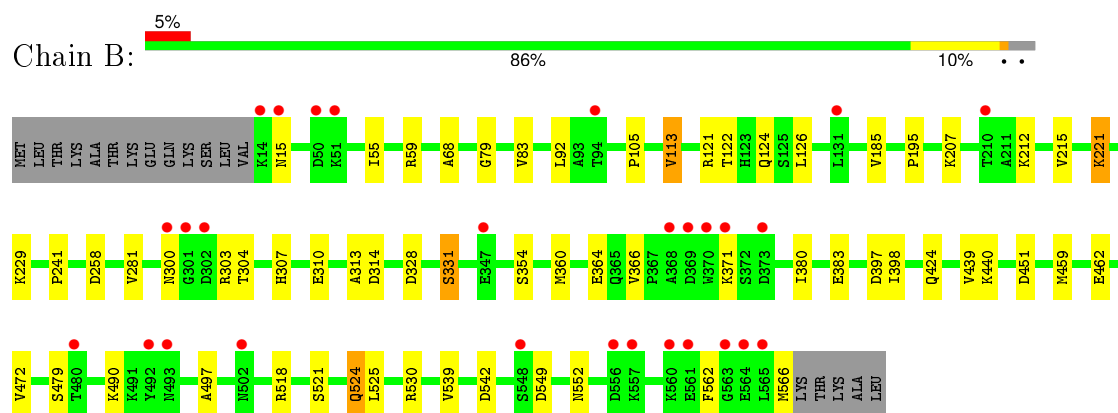
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

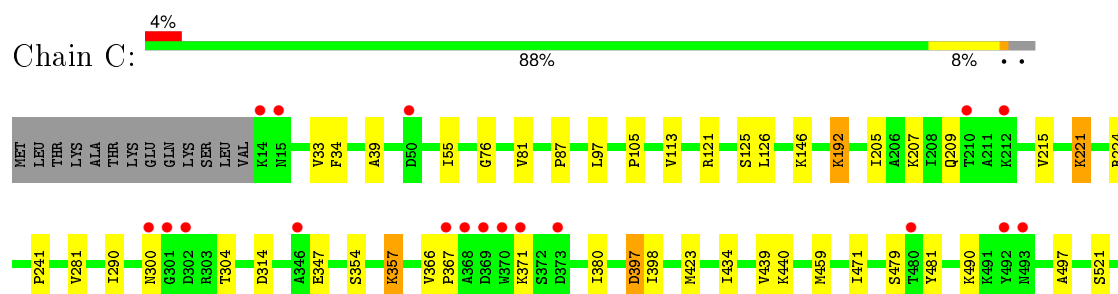
#### • Molecule 1: Acetolactate synthase

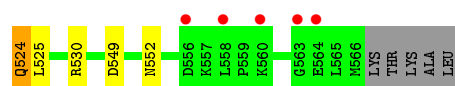


#### • Molecule 1: Acetolactate synthase

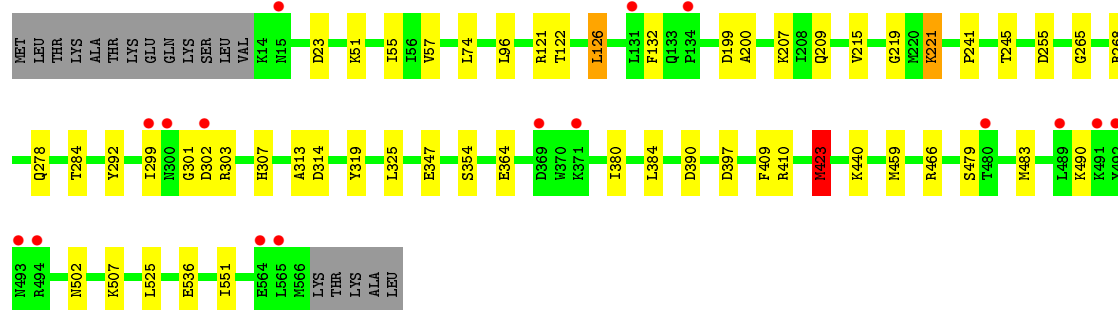
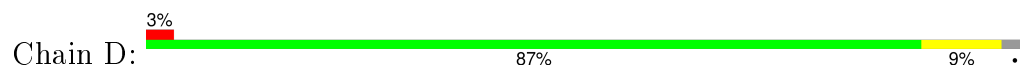


#### • Molecule 1: Acetolactate synthase

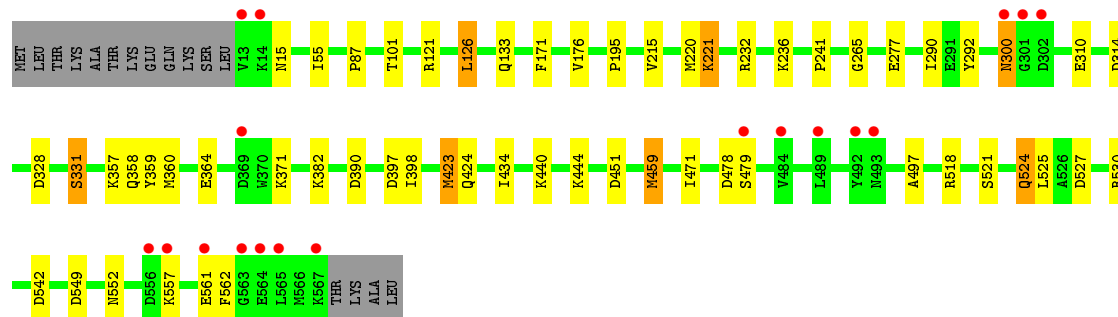
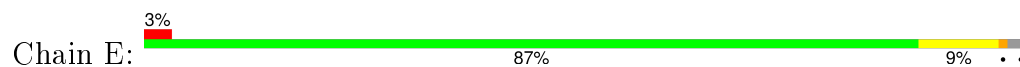




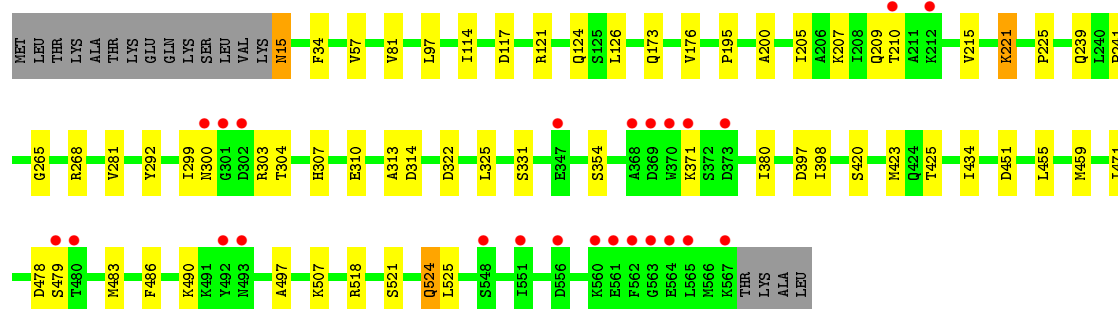
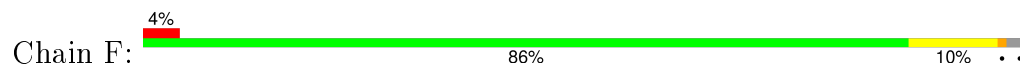
• Molecule 1: Acetolactate synthase



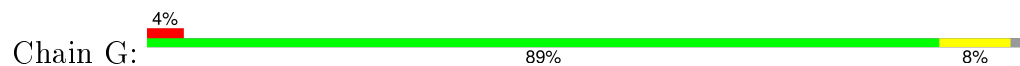
• Molecule 1: Acetolactate synthase

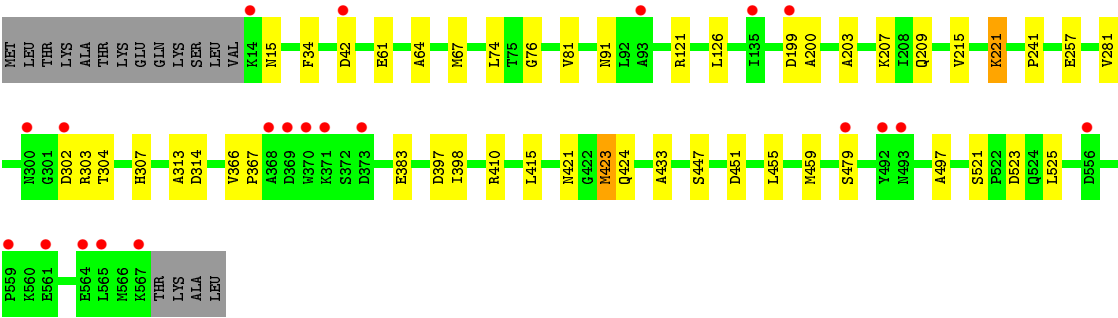


• Molecule 1: Acetolactate synthase

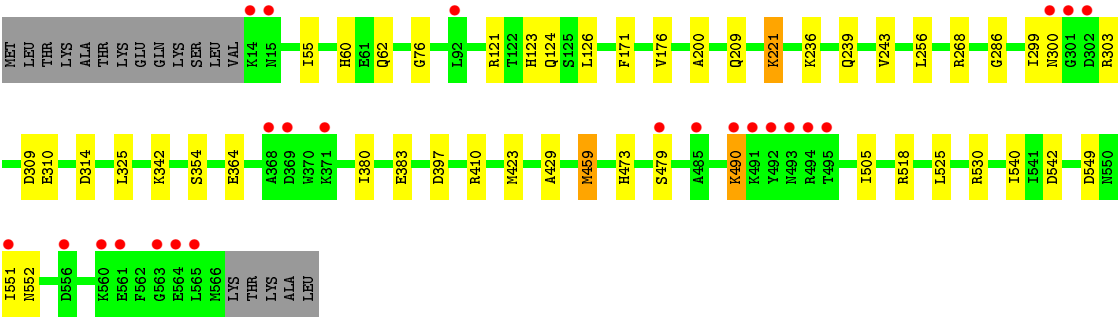
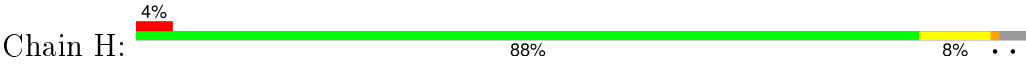


• Molecule 1: Acetolactate synthase





• Molecule 1: Acetolactate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.67Å 170.00Å 339.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.34 48.44 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.4 (30.00-2.34) 98.5 (48.44-2.34)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.172 , 0.216 0.179 , 0.221	Depositor DCC
$R_{free}$ test set	13392 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 267994 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	36626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 25.76 % 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 2.9849e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, TPP, MG, ACT

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	0.44	0/4348	0.58	0/5912
1	B	0.44	0/4340	0.58	0/5902
1	C	0.46	0/4354	0.59	0/5920
1	D	0.45	0/4385	0.59	1/5965 (0.0%)
1	E	0.45	0/4377	0.58	0/5951
1	F	0.45	0/4325	0.58	0/5881
1	G	0.44	0/4334	0.59	0/5892
1	H	0.43	0/4335	0.57	0/5894
All	All	0.45	0/34798	0.58	1/47317 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	423	MET	CG-SD-CE	-5.52	91.36	100.20

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4261	0	4280	48	0
1	B	4250	0	4264	36	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4259	0	4273	32	0
1	D	4276	0	4318	36	0
1	E	4281	0	4319	40	0
1	F	4241	0	4256	37	0
1	G	4250	0	4262	26	0
1	H	4248	0	4259	27	0
2	A	26	0	16	0	0
2	B	26	0	16	1	0
2	C	26	0	16	2	0
2	D	26	0	16	3	0
2	E	26	0	16	0	0
2	F	26	0	16	0	0
2	G	26	0	16	0	0
2	H	26	0	16	1	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
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	46	0	62	5	0
4	B	46	0	62	7	0
4	C	49	0	67	9	0
4	D	62	0	85	9	0
4	E	65	0	90	17	0
4	F	36	0	49	5	0
4	G	45	0	58	2	0
4	H	36	0	49	2	0
5	D	4	0	3	0	0
6	A	215	0	0	3	0
6	B	259	0	0	0	0
6	C	277	0	0	2	0
6	D	245	0	0	4	0
6	E	260	0	0	3	0
6	F	264	0	0	2	0
6	G	232	0	0	1	0
6	H	203	0	0	2	0
All	All	36626	0	34884	264	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 4.

The worst 5 of 264 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:101:THR:HG22	4:A:605:PG4:H82	1.61	0.83
1:D:390:ASP:H	4:D:603:PG4:H12	1.44	0.83
1:E:390:ASP:H	4:E:603:PG4:H71	1.44	0.82
1:F:398:ILE:HD11	1:F:420:SER:HB3	1.61	0.82
1:H:60:HIS:HD1	1:H:62:GLN:H	1.27	0.81

There are no symmetry-related clashes.

## 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	555/571 (97%)	544 (98%)	11 (2%)	0	100	100
1	B	554/571 (97%)	540 (98%)	13 (2%)	1 (0%)	52	61
1	C	556/571 (97%)	544 (98%)	11 (2%)	1 (0%)	52	61
1	D	560/571 (98%)	549 (98%)	10 (2%)	1 (0%)	52	61
1	E	558/571 (98%)	546 (98%)	11 (2%)	1 (0%)	52	61
1	F	552/571 (97%)	538 (98%)	13 (2%)	1 (0%)	52	61
1	G	553/571 (97%)	544 (98%)	9 (2%)	0	100	100
1	H	553/571 (97%)	542 (98%)	10 (2%)	1 (0%)	52	61
All	All	4441/4568 (97%)	4347 (98%)	88 (2%)	6 (0%)	56	67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	302	ASP
1	E	300	ASN
1	B	300	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	H	300	ASN
1	C	300	ASN

### 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	456/468 (97%)	443 (97%)	13 (3%)	50	62
1	B	455/468 (97%)	438 (96%)	17 (4%)	41	53
1	C	457/468 (98%)	442 (97%)	15 (3%)	45	57
1	D	461/468 (98%)	449 (97%)	12 (3%)	54	66
1	E	459/468 (98%)	445 (97%)	14 (3%)	47	59
1	F	453/468 (97%)	439 (97%)	14 (3%)	47	59
1	G	454/468 (97%)	444 (98%)	10 (2%)	60	73
1	H	454/468 (97%)	443 (98%)	11 (2%)	57	69
All	All	3649/3744 (98%)	3543 (97%)	106 (3%)	50	62

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	221	LYS
1	E	221	LYS
1	H	243	VAL
1	D	303	ARG
1	D	423	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	534	ASN
1	H	123	HIS
1	F	124	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	124	GLN
1	E	124	GLN

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 8 are monoatomic - leaving 41 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	601	3	20,27,27	2.00	6 (30%)	31,40,40	1.84	9 (29%)
4	PG4	A	603	-	9,9,12	0.63	0	8,8,11	0.81	0
4	PG4	A	604	-	12,12,12	0.56	0	11,11,11	0.96	1 (9%)
4	PG4	A	605	-	12,12,12	0.49	0	11,11,11	1.02	1 (9%)
4	PG4	A	606	-	9,9,12	0.63	0	8,8,11	0.97	1 (12%)
2	TPP	B	601	3	20,27,27	1.95	4 (20%)	31,40,40	1.74	10 (32%)
4	PG4	B	603	-	9,9,12	0.71	0	8,8,11	0.96	0
4	PG4	B	604	-	12,12,12	0.59	0	11,11,11	0.96	0
4	PG4	B	605	-	12,12,12	0.59	0	11,11,11	1.03	0
4	PG4	B	606	-	9,9,12	0.48	0	8,8,11	1.04	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	C	601	3	20,27,27	1.99	5 (25%)	31,40,40	2.08	11 (35%)
4	PG4	C	603	-	12,12,12	0.56	0	11,11,11	0.86	0
4	PG4	C	604	-	12,12,12	0.56	0	11,11,11	0.88	0
4	PG4	C	605	-	12,12,12	0.64	0	11,11,11	0.68	0
4	PG4	C	606	-	9,9,12	0.47	0	8,8,11	0.95	1 (12%)
2	TPP	D	601	3	20,27,27	1.96	4 (20%)	31,40,40	2.09	11 (35%)
4	PG4	D	603	-	12,12,12	0.66	0	11,11,11	0.83	0
4	PG4	D	604	-	12,12,12	0.57	0	11,11,11	0.83	0
4	PG4	D	605	-	12,12,12	0.62	0	11,11,11	0.85	0
4	PG4	D	606	-	12,12,12	0.58	0	11,11,11	0.89	0
4	PG4	D	607	-	9,9,12	0.62	0	8,8,11	0.80	0
5	ACT	D	608	-	1,3,3	1.91	0	0,3,3	0.00	-
2	TPP	E	601	3	20,27,27	2.01	5 (25%)	31,40,40	2.04	10 (32%)
4	PG4	E	603	-	12,12,12	0.70	0	11,11,11	0.99	0
4	PG4	E	604	-	12,12,12	0.57	0	11,11,11	0.96	1 (9%)
4	PG4	E	605	-	12,12,12	0.61	0	11,11,11	0.85	0
4	PG4	E	606	-	12,12,12	0.53	0	11,11,11	1.23	2 (18%)
4	PG4	E	607	-	12,12,12	0.62	0	11,11,11	0.86	0
2	TPP	F	601	3	20,27,27	1.98	7 (35%)	31,40,40	1.98	9 (29%)
4	PG4	F	603	-	12,12,12	0.62	0	11,11,11	0.95	0
4	PG4	F	604	-	12,12,12	0.65	0	11,11,11	0.92	1 (9%)
4	PG4	F	605	-	9,9,12	0.61	0	8,8,11	0.79	0
2	TPP	G	601	3	20,27,27	2.00	5 (25%)	31,40,40	1.81	10 (32%)
4	PG4	G	603	-	12,12,12	0.60	0	11,11,11	1.00	0
4	PG4	G	604	-	12,12,12	0.55	0	11,11,11	0.92	0
4	PG4	G	605	-	10,10,12	0.49	0	9,9,11	0.85	0
4	PG4	G	606	-	7,7,12	0.50	0	6,6,11	0.90	0
2	TPP	H	601	3	20,27,27	1.99	6 (30%)	31,40,40	1.91	9 (29%)
4	PG4	H	603	-	12,12,12	0.47	0	11,11,11	1.03	1 (9%)
4	PG4	H	604	-	9,9,12	0.57	0	8,8,11	0.97	1 (12%)
4	PG4	H	605	-	12,12,12	0.58	0	11,11,11	1.01	1 (9%)

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	601	3	-	0/16/17/17	0/2/2/2
4	PG4	A	603	-	-	0/7/7/10	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	A	604	-	-	0/10/10/10	0/0/0/0
4	PG4	A	605	-	-	0/10/10/10	0/0/0/0
4	PG4	A	606	-	-	0/7/7/10	0/0/0/0
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
4	PG4	B	603	-	-	0/7/7/10	0/0/0/0
4	PG4	B	604	-	-	0/10/10/10	0/0/0/0
4	PG4	B	605	-	-	0/10/10/10	0/0/0/0
4	PG4	B	606	-	-	0/7/7/10	0/0/0/0
2	TPP	C	601	3	-	0/16/17/17	0/2/2/2
4	PG4	C	603	-	-	0/10/10/10	0/0/0/0
4	PG4	C	604	-	-	0/10/10/10	0/0/0/0
4	PG4	C	605	-	-	0/10/10/10	0/0/0/0
4	PG4	C	606	-	-	0/7/7/10	0/0/0/0
2	TPP	D	601	3	-	0/16/17/17	0/2/2/2
4	PG4	D	603	-	-	0/10/10/10	0/0/0/0
4	PG4	D	604	-	-	0/10/10/10	0/0/0/0
4	PG4	D	605	-	-	0/10/10/10	0/0/0/0
4	PG4	D	606	-	-	0/10/10/10	0/0/0/0
4	PG4	D	607	-	-	0/7/7/10	0/0/0/0
5	ACT	D	608	-	-	0/0/0/0	0/0/0/0
2	TPP	E	601	3	-	0/16/17/17	0/2/2/2
4	PG4	E	603	-	-	0/10/10/10	0/0/0/0
4	PG4	E	604	-	-	0/10/10/10	0/0/0/0
4	PG4	E	605	-	-	0/10/10/10	0/0/0/0
4	PG4	E	606	-	-	0/10/10/10	0/0/0/0
4	PG4	E	607	-	-	0/10/10/10	0/0/0/0
2	TPP	F	601	3	-	0/16/17/17	0/2/2/2
4	PG4	F	603	-	-	0/10/10/10	0/0/0/0
4	PG4	F	604	-	-	0/10/10/10	0/0/0/0
4	PG4	F	605	-	-	0/7/7/10	0/0/0/0
2	TPP	G	601	3	-	0/16/17/17	0/2/2/2
4	PG4	G	603	-	-	0/10/10/10	0/0/0/0
4	PG4	G	604	-	-	0/10/10/10	0/0/0/0
4	PG4	G	605	-	-	0/8/8/10	0/0/0/0
4	PG4	G	606	-	-	0/5/5/10	0/0/0/0
2	TPP	H	601	3	-	0/16/17/17	0/2/2/2
4	PG4	H	603	-	-	0/10/10/10	0/0/0/0
4	PG4	H	604	-	-	0/7/7/10	0/0/0/0
4	PG4	H	605	-	-	0/10/10/10	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	TPP	C4-N3	-5.05	1.35	1.39
2	A	601	TPP	C4-N3	-5.04	1.35	1.39
2	G	601	TPP	C4-N3	-4.97	1.35	1.39
2	E	601	TPP	C4-N3	-4.74	1.35	1.39
2	D	601	TPP	C4-N3	-4.71	1.35	1.39

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TPP	N1'-C2'-N3'	-3.96	118.28	125.60
2	D	601	TPP	CM4-C4-C5	-3.95	120.03	128.90
2	C	601	TPP	CM4-C4-C5	-3.94	120.05	128.90
2	H	601	TPP	CM4-C4-C5	-3.84	120.27	128.90
2	F	601	TPP	CM4-C4-C5	-3.80	120.36	128.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

26 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	PG4	1	0
4	A	604	PG4	3	0
4	A	605	PG4	1	0
2	B	601	TPP	1	0
4	B	603	PG4	2	0
4	B	605	PG4	4	0
4	B	606	PG4	1	0
2	C	601	TPP	2	0
4	C	603	PG4	1	0
4	C	604	PG4	2	0
4	C	605	PG4	4	0
4	C	606	PG4	2	0
2	D	601	TPP	3	0
4	D	603	PG4	1	0
4	D	604	PG4	1	0
4	D	605	PG4	2	0
4	D	606	PG4	3	0
4	D	607	PG4	2	0
4	E	603	PG4	9	0
4	E	606	PG4	6	0
4	E	607	PG4	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	603	PG4	4	0
4	F	604	PG4	1	0
4	G	603	PG4	2	0
2	H	601	TPP	1	0
4	H	605	PG4	2	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	555/571 (97%)	-0.11	22 (3%)	42	54	11, 23, 45, 79	0
1	B	553/571 (96%)	0.04	28 (5%)	32	45	9, 20, 44, 72	0
1	C	553/571 (96%)	0.03	23 (4%)	40	52	11, 19, 40, 71	0
1	D	553/571 (96%)	-0.17	16 (2%)	55	66	10, 20, 43, 70	0
1	E	555/571 (97%)	-0.19	18 (3%)	51	62	9, 19, 42, 71	0
1	F	553/571 (96%)	0.00	25 (4%)	37	50	11, 20, 42, 68	0
1	G	554/571 (97%)	0.01	21 (3%)	44	56	11, 21, 43, 76	0
1	H	553/571 (96%)	-0.10	24 (4%)	39	51	13, 24, 47, 71	0
All	All	4429/4568 (96%)	-0.06	177 (3%)	42	54	9, 21, 44, 79	0

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	568	THR	8.0
1	E	300	ASN	7.0
1	D	564	GLU	4.5
1	A	493	ASN	4.5
1	A	492	TYR	4.4

### 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	PG4	B	606	10/13	0.84	0.22	8.70	33,45,50,58	0
4	PG4	D	603	13/13	0.88	0.19	8.40	20,27,37,42	0
4	PG4	E	606	13/13	0.85	0.24	5.46	18,31,41,42	0
4	PG4	E	605	13/13	0.85	0.19	3.98	33,46,53,58	0
4	PG4	A	605	13/13	0.85	0.17	3.78	28,37,48,48	0
4	PG4	F	603	13/13	0.94	0.24	3.68	25,31,38,40	0
5	ACT	D	608	4/4	0.85	0.15	3.55	30,32,34,37	0
4	PG4	E	603	13/13	0.91	0.19	3.38	24,30,36,40	0
4	PG4	B	605	13/13	0.93	0.20	2.97	24,29,39,44	0
4	PG4	H	605	13/13	0.87	0.20	2.76	26,37,46,50	0
4	PG4	C	606	10/13	0.84	0.21	2.76	36,48,52,55	0
4	PG4	E	607	13/13	0.92	0.19	2.42	37,47,58,59	0
4	PG4	G	604	13/13	0.93	0.19	2.28	22,29,41,41	0
4	PG4	G	606	8/13	0.83	0.19	2.10	41,46,52,53	0
4	PG4	H	604	10/13	0.89	0.15	1.73	36,42,48,52	0
4	PG4	D	605	13/13	0.95	0.18	1.48	22,30,49,52	0
4	PG4	A	603	10/13	0.96	0.14	1.41	21,29,38,40	0
4	PG4	H	603	13/13	0.79	0.21	1.17	28,40,48,50	0
4	PG4	G	605	11/13	0.86	0.15	1.00	31,39,47,52	0
4	PG4	D	606	13/13	0.95	0.17	0.98	26,33,38,43	0
4	PG4	D	604	13/13	0.92	0.17	0.92	23,32,42,46	0
4	PG4	E	604	13/13	0.86	0.17	0.89	37,49,60,74	0
4	PG4	B	604	13/13	0.91	0.16	0.83	37,42,51,59	0
4	PG4	G	603	13/13	0.90	0.15	0.60	17,31,49,49	0
4	PG4	C	605	13/13	0.95	0.15	0.43	16,28,41,41	0
4	PG4	B	603	10/13	0.95	0.13	0.29	13,24,31,42	0
4	PG4	D	607	10/13	0.91	0.12	0.23	31,39,47,49	0
2	TPP	D	601	26/26	0.95	0.14	0.21	15,27,35,41	0
4	PG4	F	605	10/13	0.89	0.13	0.16	34,40,43,48	0
4	PG4	A	604	13/13	0.92	0.13	0.16	27,35,47,47	0
2	TPP	A	601	26/26	0.93	0.14	0.14	19,30,38,38	0
2	TPP	E	601	26/26	0.96	0.13	0.13	15,24,35,35	0
4	PG4	C	603	13/13	0.96	0.17	0.10	21,27,34,36	0
4	PG4	F	604	13/13	0.94	0.13	0.09	19,29,41,42	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	PG4	C	604	13/13	0.91	0.13	0.05	32,37,47,49	0
4	PG4	A	606	10/13	0.94	0.10	0.02	36,41,45,47	0
2	TPP	H	601	26/26	0.94	0.13	-0.12	17,28,36,39	0
3	MG	H	602	1/1	0.96	0.16	-0.38	36,36,36,36	0
2	TPP	F	601	26/26	0.94	0.13	-0.47	17,27,33,34	0
2	TPP	C	601	26/26	0.95	0.12	-0.47	13,27,33,34	0
2	TPP	G	601	26/26	0.95	0.12	-0.74	17,25,32,35	0
2	TPP	B	601	26/26	0.96	0.11	-0.80	17,29,33,36	0
3	MG	E	602	1/1	0.97	0.11	-0.93	30,30,30,30	0
3	MG	F	602	1/1	0.98	0.10	-0.98	24,24,24,24	0
3	MG	B	602	1/1	0.96	0.06	-1.60	29,29,29,29	0
3	MG	A	602	1/1	0.98	0.05	-1.73	29,29,29,29	0
3	MG	C	602	1/1	0.94	0.04	-1.76	28,28,28,28	0
3	MG	D	602	1/1	0.98	0.06	-1.79	25,25,25,25	0
3	MG	G	602	1/1	0.97	0.05	-2.23	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.