



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 07:30 am BST

PDB ID : 1GU1  
Title : Crystal structure of type II dehydroquinase from *Streptomyces coelicolor* complexed with 2,3-anhydro-quinic acid  
Authors : Roszak, A.W.; Robinson, D.A.; Krell, T.; Hunter, I.S.; Coggins, J.R.; Laphorn, A.J.  
Deposited on : 2002-01-22  
Resolution : 1.80 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

<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)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

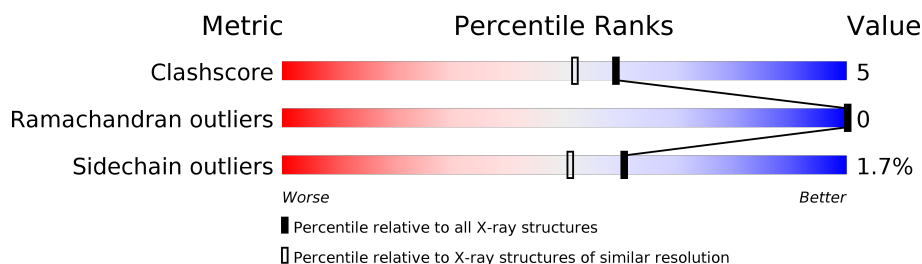
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	87% 7% . .
1	B	156	85% 9% . .
1	C	156	87% 7% . .
1	D	156	85% 7% . .
1	E	156	87% 7% . .
1	F	156	89% 5% . .
1	G	156	86% 8% . .
1	H	156	88% 5% . .

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Mol	Chain	Length	Quality of chain
1	I	156	<div><div></div><div>87%</div><div>8% . .</div></div>
1	J	156	<div><div></div><div>86%</div><div>8% . .</div></div>
1	K	156	<div><div></div><div>88%</div><div>. . .</div></div>
1	L	156	<div><div></div><div>90%</div><div>. . .</div></div>

## 2 Entry composition

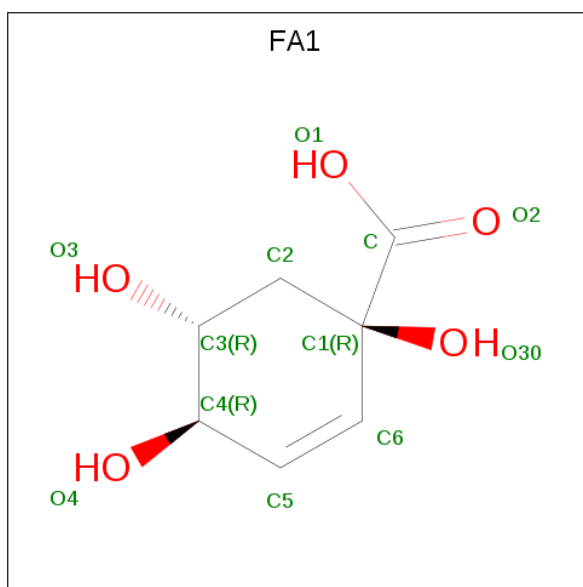
There are 6 unique types of molecules in this entry. The entry contains 16578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	B	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	C	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	D	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	E	149	Total	C	N	O	S	0	4	0
			1134	705	210	214	5			
1	F	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	G	149	Total	C	N	O	S	0	4	0
			1134	705	210	214	5			
1	H	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	I	149	Total	C	N	O	S	0	2	0
			1126	700	209	212	5			
1	J	149	Total	C	N	O	S	0	3	0
			1130	702	209	214	5			
1	K	149	Total	C	N	O	S	0	4	0
			1136	705	212	214	5			
1	L	149	Total	C	N	O	S	0	4	0
			1136	705	212	214	5			

- Molecule 2 is 2,3 -ANHYDRO-QUINIC ACID (three-letter code: FA1) (formula: C<sub>7</sub>H<sub>10</sub>O<sub>5</sub>).



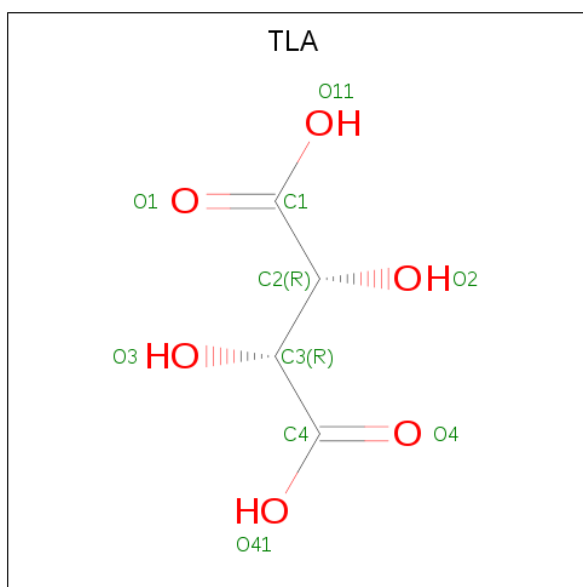
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	7	5		
2	B	1	Total	C	O	0	0
			12	7	5		
2	C	1	Total	C	O	0	0
			12	7	5		
2	D	1	Total	C	O	0	0
			12	7	5		
2	E	1	Total	C	O	0	0
			12	7	5		
2	F	1	Total	C	O	0	0
			12	7	5		
2	G	1	Total	C	O	0	0
			12	7	5		
2	H	1	Total	C	O	0	0
			12	7	5		
2	I	1	Total	C	O	0	0
			12	7	5		
2	J	1	Total	C	O	0	0
			12	7	5		
2	K	1	Total	C	O	0	0
			12	7	5		
2	L	1	Total	C	O	0	0
			12	7	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



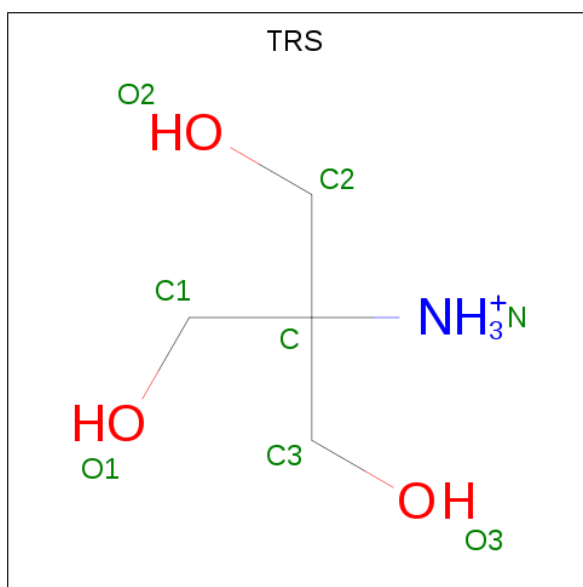
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	4	6		
4	B	1	Total	C	O	0	0
			10	4	6		
4	C	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		
4	E	1	Total	C	O	0	0
			10	4	6		
4	F	1	Total	C	O	0	0
			10	4	6		
4	G	1	Total	C	O	0	0
			10	4	6		
4	H	1	Total	C	O	0	0
			10	4	6		
4	I	1	Total	C	O	0	0
			10	4	6		
4	J	1	Total	C	O	0	0
			10	4	6		
4	K	1	Total	C	O	0	0
			10	4	6		
4	L	1	Total	C	O	0	0
			10	4	6		

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	H	1	Total	C	N	O	0	0
			8	4	1	3		
5	L	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	233	Total	O	0	0
			233	233		
6	B	226	Total	O	0	0
			226	226		
6	C	191	Total	O	0	0
			191	191		
6	D	215	Total	O	0	0
			215	215		
6	E	238	Total	O	0	0
			238	238		
6	F	235	Total	O	0	0
			235	235		
6	G	245	Total	O	0	0
			245	245		
6	H	231	Total	O	0	0
			231	231		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	215	Total 215	O 215	0	0
6	J	199	Total 199	O 199	0	0
6	K	221	Total 221	O 221	0	0
6	L	185	Total 185	O 185	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.


Note EDS was not executed.

#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A: 



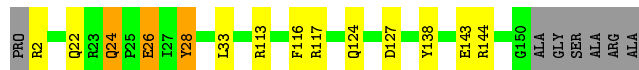
#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B: 



#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C: 



#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D: 




#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain E: 




#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:  89% 5% . .



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:  86% 8% . .




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:  88% 5% . .




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:  87% 8% . .




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  86% 8% . .




• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  88% . . .



• Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:  90% . . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.60Å 138.40Å 141.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.00 – 1.80	Depositor
% Data completeness (in resolution range)	98.1 (22.00-1.80)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.155 , 0.200	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16578	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 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: GOL, TLA, FA1, TRS

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	0.76	0/1168	1.42	8/1591 (0.5%)
1	B	0.77	0/1168	1.40	11/1591 (0.7%)
1	C	0.79	0/1168	1.50	12/1591 (0.8%)
1	D	0.85	0/1168	1.57	19/1591 (1.2%)
1	E	0.80	0/1177	1.52	12/1602 (0.7%)
1	F	0.80	0/1168	1.42	8/1591 (0.5%)
1	G	0.80	0/1177	1.55	12/1602 (0.7%)
1	H	0.79	0/1168	1.45	9/1591 (0.6%)
1	I	0.78	0/1159	1.44	11/1579 (0.7%)
1	J	0.84	0/1168	1.73	16/1591 (1.0%)
1	K	0.80	0/1179	1.49	10/1605 (0.6%)
1	L	0.78	0/1179	1.42	5/1605 (0.3%)
All	All	0.80	0/14047	1.49	133/19130 (0.7%)

There are no bond length outliers.

The worst 5 of 133 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	144	ARG	NE-CZ-NH2	-24.13	108.24	120.30
1	K	144	ARG	NE-CZ-NH2	-22.53	109.03	120.30
1	H	144	ARG	NE-CZ-NH2	-22.36	109.12	120.30
1	J	144	ARG	NE-CZ-NH2	-21.08	109.76	120.30
1	J	2	ARG	CD-NE-CZ	19.89	151.44	123.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1130	0	1096	11	0
1	B	1130	0	1096	9	1
1	C	1130	0	1096	12	0
1	D	1130	0	1096	11	0
1	E	1134	0	1105	13	0
1	F	1130	0	1096	12	0
1	G	1134	0	1105	10	0
1	H	1130	0	1096	11	1
1	I	1126	0	1094	7	0
1	J	1130	0	1096	13	0
1	K	1136	0	1106	14	0
1	L	1136	0	1106	7	0
2	A	12	0	9	0	0
2	B	12	0	7	0	0
2	C	12	0	7	0	0
2	D	12	0	7	0	0
2	E	12	0	7	0	0
2	F	12	0	9	0	0
2	G	12	0	8	0	0
2	H	12	0	7	0	0
2	I	12	0	8	0	0
2	J	12	0	7	0	0
2	K	12	0	7	0	0
2	L	12	0	7	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	E	6	0	8	0	0
3	F	6	0	8	0	0
3	G	6	0	8	0	0
3	H	6	0	8	0	0
3	I	6	0	8	0	0
3	J	6	0	8	0	0
3	K	6	0	8	0	0
3	L	6	0	8	0	0
4	A	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	10	0	4	0	0
4	C	10	0	4	1	0
4	D	10	0	4	1	0
4	E	10	0	4	1	0
4	F	10	0	4	0	0
4	G	10	0	4	0	0
4	H	10	0	4	1	0
4	I	10	0	4	0	0
4	J	10	0	4	0	0
4	K	10	0	4	1	0
4	L	10	0	4	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	H	8	0	12	0	0
5	L	8	0	12	0	0
6	A	233	0	0	7	0
6	B	226	0	0	5	0
6	C	191	0	0	5	0
6	D	215	0	0	7	0
6	E	238	0	0	10	0
6	F	235	0	0	8	0
6	G	245	0	0	7	0
6	H	231	0	0	9	0
6	I	215	0	0	7	0
6	J	199	0	0	12	0
6	K	221	0	0	6	0
6	L	185	0	0	3	0
All	All	16578	0	13470	129	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.

The worst 5 of 129 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:E:124[B]:GLN:CG	6:E:2212:HOH:O	1.68	1.34
1:F:124[A]:GLN:NE2	6:F:2207:HOH:O	1.62	1.29
1:J:124[B]:GLN:HG3	6:J:2173:HOH:O	1.29	1.28
1:A:124[B]:GLN:HG3	6:A:2196:HOH:O	1.15	1.28
1:D:124[B]:GLN:NE2	6:D:2190:HOH:O	1.61	1.25

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:B:68:GLU:OE2	1:H:6:ASN:ND2[4_456]	1.97	0.23

## 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	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	B	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	C	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	D	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	E	151/156 (97%)	148 (98%)	3 (2%)	0	100	100
1	F	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	G	151/156 (97%)	148 (98%)	3 (2%)	0	100	100
1	H	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	I	149/156 (96%)	146 (98%)	3 (2%)	0	100	100
1	J	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	K	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
1	L	150/156 (96%)	147 (98%)	3 (2%)	0	100	100
All	All	1801/1872 (96%)	1765 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	B	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	C	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	D	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	E	121/120 (101%)	119 (98%)	2 (2%)	60	51
1	F	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	G	121/120 (101%)	119 (98%)	2 (2%)	60	51
1	H	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	I	119/120 (99%)	117 (98%)	2 (2%)	60	51
1	J	120/120 (100%)	118 (98%)	2 (2%)	60	51
1	K	121/120 (101%)	119 (98%)	2 (2%)	60	51
1	L	121/120 (101%)	119 (98%)	2 (2%)	60	51
All	All	1443/1440 (100%)	1419 (98%)	24 (2%)	60	51

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	24	GLN
1	G	26	GLU
1	L	24	GLN
1	F	26	GLU
1	G	24	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	22	GLN
1	G	24	GLN
1	K	24	GLN
1	F	24	GLN
1	G	22	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 ⓘ

40 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	TLA	C	203	-	3,9,9	0.42	0	6,12,12	1.52	1 (16%)
2	FA1	K	201	-	7,12,12	6.05	6 (85%)	7,18,18	1.74	1 (14%)
5	TRS	H	204	-	7,7,7	0.93	0	9,9,9	0.62	0
3	GOL	H	202	-	5,5,5	0.95	0	5,5,5	0.79	0
3	GOL	J	202	-	5,5,5	1.52	1 (20%)	5,5,5	0.78	0
2	FA1	F	201	-	7,12,12	6.01	6 (85%)	7,18,18	1.65	1 (14%)
4	TLA	D	203	-	3,9,9	0.81	0	6,12,12	1.29	1 (16%)
4	TLA	K	203	-	3,9,9	0.44	0	6,12,12	1.21	1 (16%)
2	FA1	H	201	-	7,12,12	5.63	7 (100%)	7,18,18	1.71	1 (14%)
2	FA1	J	201	-	7,12,12	5.34	7 (100%)	7,18,18	1.42	2 (28%)
3	GOL	G	202	-	5,5,5	1.15	1 (20%)	5,5,5	0.48	0
4	TLA	A	203	-	3,9,9	0.52	0	6,12,12	1.46	1 (16%)
4	TLA	H	203	-	3,9,9	0.83	0	6,12,12	1.17	0
4	TLA	J	203	-	3,9,9	0.61	0	6,12,12	1.12	0
4	TLA	F	203	-	3,9,9	0.59	0	6,12,12	1.55	1 (16%)
3	GOL	D	202	-	5,5,5	0.97	0	5,5,5	0.71	0
2	FA1	B	201	-	7,12,12	4.66	7 (100%)	7,18,18	1.30	1 (14%)
4	TLA	E	203	-	3,9,9	0.45	0	6,12,12	1.14	1 (16%)
2	FA1	G	201	-	7,12,12	5.49	6 (85%)	7,18,18	1.62	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	TLA	L	203	-	3,9,9	0.49	0	6,12,12	0.94	0
3	GOL	E	202	-	5,5,5	1.21	1 (20%)	5,5,5	0.76	0
5	TRS	A	204	-	7,7,7	1.05	0	9,9,9	0.47	0
3	GOL	F	202	-	5,5,5	0.83	0	5,5,5	0.49	0
2	FA1	L	201	-	7,12,12	5.08	7 (100%)	7,18,18	1.36	2 (28%)
2	FA1	A	201	-	7,12,12	5.94	7 (100%)	7,18,18	1.25	1 (14%)
3	GOL	I	202	-	5,5,5	1.14	1 (20%)	5,5,5	0.71	0
3	GOL	K	202	-	5,5,5	1.28	1 (20%)	5,5,5	0.56	0
5	TRS	B	204	-	7,7,7	0.79	0	9,9,9	0.78	0
2	FA1	I	201	-	7,12,12	5.93	7 (100%)	7,18,18	1.84	1 (14%)
3	GOL	A	202	-	5,5,5	0.95	0	5,5,5	0.49	0
2	FA1	D	201	-	7,12,12	5.51	7 (100%)	7,18,18	1.20	0
4	TLA	G	203	-	3,9,9	0.42	0	6,12,12	1.53	2 (33%)
3	GOL	L	202	-	5,5,5	0.86	0	5,5,5	0.43	0
4	TLA	B	203	-	3,9,9	0.99	0	6,12,12	1.01	0
4	TLA	I	203	-	3,9,9	0.49	0	6,12,12	1.09	0
5	TRS	L	204	-	7,7,7	0.80	0	9,9,9	0.58	0
3	GOL	B	202	-	5,5,5	1.20	1 (20%)	5,5,5	0.44	0
2	FA1	C	201	-	7,12,12	5.24	7 (100%)	7,18,18	2.26	2 (28%)
3	GOL	C	202	-	5,5,5	1.14	1 (20%)	5,5,5	0.84	0
2	FA1	E	201	-	7,12,12	6.02	7 (100%)	7,18,18	1.47	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLA	C	203	-	-	0/4/12/12	-
2	FA1	K	201	-	-	0/0/21/21	0/1/1/1
5	TRS	H	204	-	-	0/9/9/9	-
3	GOL	H	202	-	-	1/4/4/4	-
3	GOL	J	202	-	-	0/4/4/4	-
2	FA1	F	201	-	-	0/0/21/21	0/1/1/1
4	TLA	D	203	-	-	0/4/12/12	-
4	TLA	K	203	-	-	0/4/12/12	-
2	FA1	H	201	-	-	0/0/21/21	0/1/1/1
2	FA1	J	201	-	-	0/0/21/21	0/1/1/1
3	GOL	G	202	-	-	0/4/4/4	-
4	TLA	A	203	-	-	0/4/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TLA	H	203	-	-	0/4/12/12	-
4	TLA	J	203	-	-	0/4/12/12	-
4	TLA	F	203	-	-	0/4/12/12	-
3	GOL	D	202	-	-	0/4/4/4	-
2	FA1	B	201	-	-	0/0/21/21	0/1/1/1
4	TLA	E	203	-	-	0/4/12/12	-
2	FA1	G	201	-	-	0/0/21/21	0/1/1/1
4	TLA	L	203	-	-	0/4/12/12	-
3	GOL	E	202	-	-	0/4/4/4	-
5	TRS	A	204	-	-	0/9/9/9	-
3	GOL	F	202	-	-	1/4/4/4	-
2	FA1	L	201	-	-	0/0/21/21	0/1/1/1
2	FA1	A	201	-	-	0/0/21/21	0/1/1/1
3	GOL	I	202	-	-	0/4/4/4	-
3	GOL	K	202	-	-	1/4/4/4	-
5	TRS	B	204	-	-	0/9/9/9	-
2	FA1	I	201	-	-	0/0/21/21	0/1/1/1
3	GOL	A	202	-	-	1/4/4/4	-
2	FA1	D	201	-	-	0/0/21/21	0/1/1/1
4	TLA	G	203	-	-	0/4/12/12	-
3	GOL	L	202	-	-	0/4/4/4	-
4	TLA	B	203	-	-	0/4/12/12	-
4	TLA	I	203	-	-	0/4/12/12	-
5	TRS	L	204	-	-	0/9/9/9	-
3	GOL	B	202	-	-	0/4/4/4	-
2	FA1	C	201	-	-	0/0/21/21	0/1/1/1
3	GOL	C	202	-	-	0/4/4/4	-
2	FA1	E	201	-	-	0/0/21/21	0/1/1/1

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	201	FA1	C1-C6	-11.99	1.39	1.50
2	F	201	FA1	C1-C6	-11.83	1.39	1.50
2	K	201	FA1	C1-C6	-11.45	1.40	1.50
2	E	201	FA1	C1-C6	-11.16	1.40	1.50
2	A	201	FA1	C1-C6	-11.05	1.40	1.50

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FA1	O4-C4-C3	4.97	118.04	109.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	FA1	O4-C4-C3	4.17	116.66	109.42
2	F	201	FA1	O4-C4-C3	3.96	116.29	109.42
2	H	201	FA1	O4-C4-C3	3.83	116.06	109.42
2	K	201	FA1	C4-C5-C6	-3.47	119.23	123.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	202	GOL	C1-C2-C3-O3
3	A	202	GOL	C1-C2-C3-O3
3	H	202	GOL	C1-C2-C3-O3
3	K	202	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	203	TLA	1	0
4	D	203	TLA	1	0
4	K	203	TLA	1	0
4	H	203	TLA	1	0
4	E	203	TLA	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.