



wwPDB X-ray Structure Validation Summary Report

Dec 8, 2023 – 12:53 am GMT

PDB ID : 1GTZ
Title : Structure of STREPTOMYCES COELICOLOR TYPE II DEHYDRO-
QUINASE R23A MUTANT IN COMPLEX WITH DEHYDROSHIKIMATE
Authors : Roszak, A.W.; Krell, T.; Robinson, D.A.; Hunter, I.S.; Coggins, J.R.;
Laphorn, A.J.
Deposited on : 2002-01-22
Resolution : 1.60 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
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) : 2.36

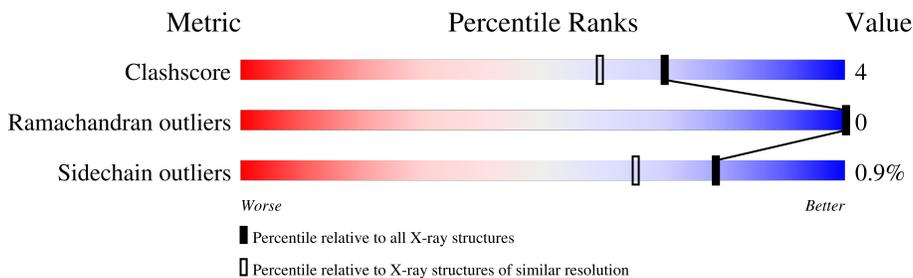
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 ≥ 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	
1	B	156	
1	C	156	
1	D	156	
1	E	156	
1	F	156	
1	G	156	
1	H	156	

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Mol	Chain	Length	Quality of chain
1	I	156	 83% 12% . .
1	J	156	 74% 19% . . .
1	K	156	 81% 13% . . .
1	L	156	 80% 14% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15328 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
			Total	C	N	O	S			
1	A	149	1131	704	206	215	6	0	6	0
1	B	149	1131	704	206	215	6	0	6	0
1	C	149	1131	704	206	215	6	0	6	0
1	D	149	1131	704	206	215	6	0	6	0
1	E	149	1131	704	206	215	6	0	6	0
1	F	149	1131	704	206	215	6	0	6	0
1	G	149	1131	704	206	215	6	0	6	0
1	H	149	1131	704	206	215	6	0	6	0
1	I	149	1131	704	206	215	6	0	6	0
1	J	149	1131	704	206	215	6	0	6	0
1	K	149	1131	704	206	215	6	0	6	0
1	L	149	1131	704	206	215	6	0	6	0

There are 12 discrepancies between the modelled and reference sequences:

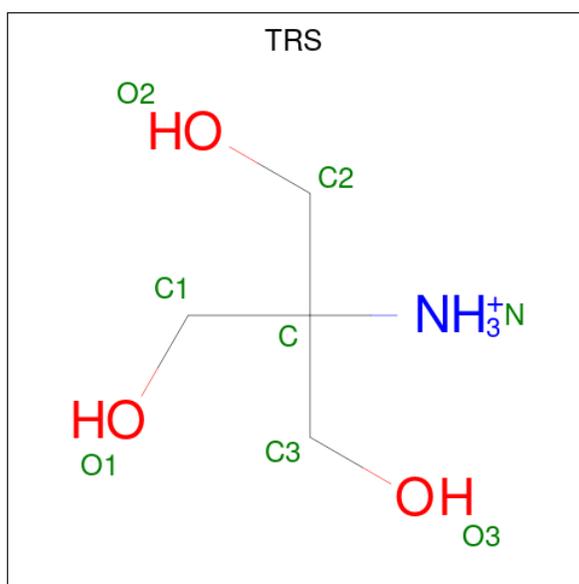
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	ARG	engineered mutation	UNP P15474
B	23	ALA	ARG	engineered mutation	UNP P15474
C	23	ALA	ARG	engineered mutation	UNP P15474
D	23	ALA	ARG	engineered mutation	UNP P15474
E	23	ALA	ARG	engineered mutation	UNP P15474

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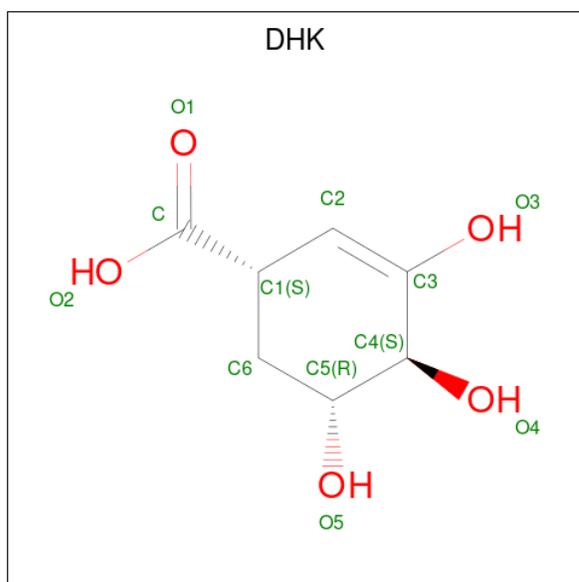
Chain	Residue	Modelled	Actual	Comment	Reference
F	23	ALA	ARG	engineered mutation	UNP P15474
G	23	ALA	ARG	engineered mutation	UNP P15474
H	23	ALA	ARG	engineered mutation	UNP P15474
I	23	ALA	ARG	engineered mutation	UNP P15474
J	23	ALA	ARG	engineered mutation	UNP P15474
K	23	ALA	ARG	engineered mutation	UNP P15474
L	23	ALA	ARG	engineered mutation	UNP P15474

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is 3-DEHYDROSHIKIMATE (three-letter code: DHK) (formula: C₇H₁₀O₅).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	140	Total O 140 140	0	0
4	B	116	Total O 116 116	0	0
4	C	93	Total O 93 93	0	0
4	D	137	Total O 137 137	0	0
4	E	163	Total O 163 163	0	0
4	F	135	Total O 135 135	0	0
4	G	154	Total O 154 154	0	0
4	H	140	Total O 140 140	0	0
4	I	153	Total O 153 153	0	0
4	J	109	Total O 109 109	0	0
4	K	134	Total O 134 134	0	0
4	L	106	Total O 106 106	0	0

3 Residue-property plots

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. 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: 



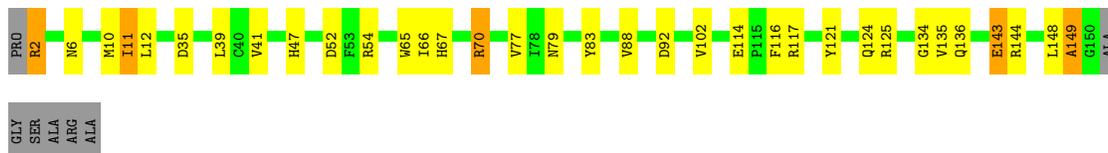
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

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:  81% 12% ..



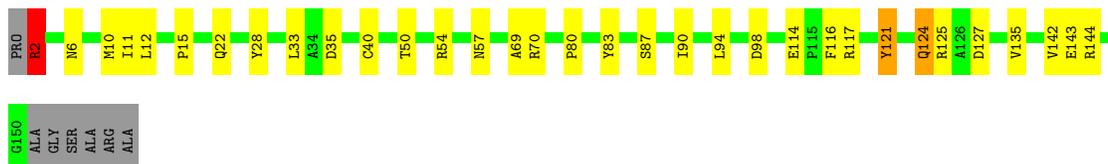
- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:  81% 13% ..



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:  74% 19% ..



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:  83% 12% ..



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  74% 19% ..



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  81% 13% ..



- Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:  80% 14% ..



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.10Å 136.20Å 96.70Å 90.00° 101.28° 90.00°	Depositor
Resolution (Å)	45.00 – 1.60	Depositor
% Data completeness (in resolution range)	73.8 (45.00-1.60)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15328	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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: TRS, DHK

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	1.08	1/1184 (0.1%)	1.76	19/1613 (1.2%)
1	B	1.07	1/1184 (0.1%)	1.68	22/1613 (1.4%)
1	C	1.23	1/1184 (0.1%)	1.94	34/1613 (2.1%)
1	D	1.08	0/1184	1.66	16/1613 (1.0%)
1	E	1.12	0/1184	1.70	20/1613 (1.2%)
1	F	1.05	0/1184	1.72	18/1613 (1.1%)
1	G	1.07	0/1184	1.69	15/1613 (0.9%)
1	H	1.06	1/1184 (0.1%)	1.79	29/1613 (1.8%)
1	I	1.06	0/1184	1.82	20/1613 (1.2%)
1	J	1.19	3/1184 (0.3%)	1.95	33/1613 (2.0%)
1	K	1.11	0/1184	1.63	14/1613 (0.9%)
1	L	1.02	0/1184	1.74	21/1613 (1.3%)
All	All	1.10	7/14208 (0.0%)	1.76	261/19356 (1.3%)

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	1
1	C	0	2
1	D	0	1
1	F	0	2
1	H	0	1
1	L	0	1
All	All	0	8

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	60	GLY	CA-C	5.57	1.60	1.51
1	A	114	GLU	CD-OE1	5.39	1.31	1.25
1	C	136	GLN	C-N	5.20	1.42	1.33
1	B	59	GLU	CD-OE1	5.19	1.31	1.25
1	H	87	SER	CB-OG	-5.16	1.35	1.42

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	144	ARG	NE-CZ-NH1	-25.52	107.54	120.30
1	A	2	ARG	CD-NE-CZ	19.50	150.91	123.60
1	I	2	ARG	NE-CZ-NH1	-17.70	111.45	120.30
1	A	2	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	J	117	ARG	NE-CZ-NH2	-16.13	112.23	120.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	SER	Mainchain
1	C	135	VAL	Mainchain
1	C	149	ALA	Mainchain
1	D	89	ALA	Mainchain
1	F	83	TYR	Mainchain

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	1131	0	1101	4	0
1	B	1131	0	1101	10	0
1	C	1131	0	1101	8	0
1	D	1131	0	1101	8	0
1	E	1131	0	1101	11	0
1	F	1131	0	1101	7	1
1	G	1131	0	1101	8	0
1	H	1131	0	1101	13	1
1	I	1131	0	1101	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1131	0	1100	9	0
1	K	1131	0	1101	9	0
1	L	1131	0	1101	4	1
2	A	8	0	12	0	0
2	D	8	0	12	0	0
2	G	8	0	12	0	0
2	J	8	0	12	0	0
3	A	12	0	6	0	0
3	B	12	0	6	0	0
3	C	12	0	7	0	0
3	D	12	0	7	0	0
3	E	12	0	6	0	0
3	F	12	0	6	0	0
3	G	12	0	7	0	0
3	H	12	0	8	0	0
3	I	12	0	6	0	0
3	J	12	0	7	0	0
3	K	12	0	6	0	0
3	L	12	0	5	0	0
4	A	140	0	0	0	2
4	B	116	0	0	2	0
4	C	93	0	0	0	0
4	D	137	0	0	2	0
4	E	163	0	0	1	3
4	F	135	0	0	2	2
4	G	154	0	0	2	2
4	H	140	0	0	2	0
4	I	153	0	0	2	2
4	J	109	0	0	0	0
4	K	134	0	0	2	3
4	L	106	0	0	0	0
All	All	15328	0	13336	97	9

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 97 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:H:22:GLN:NE2	4:H:2027:HOH:O	1.98	0.94
1:J:10[B]:MET:SD	1:J:12:LEU:HD21	2.18	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143[B]:GLU:OE1	4:D:2133:HOH:O	1.99	0.80
1:A:10[B]:MET:SD	1:A:69:ALA:HB2	2.22	0.80
1:H:2:ARG:HG2	1:H:2:ARG:HH21	1.49	0.75

The worst 5 of 9 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)
4:E:2027:HOH:O	4:K:2066:HOH:O[2_645]	1.43	0.77
4:F:2047:HOH:O	4:I:2053:HOH:O[2_545]	1.69	0.51
4:E:2012:HOH:O	4:K:2023:HOH:O[2_645]	1.74	0.46
1:F:22:GLN:NE2	1:I:6:ASN:O[2_545]	1.84	0.36
4:F:2048:HOH:O	4:I:2025:HOH:O[2_545]	2.03	0.17

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	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	B	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
1	C	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	D	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	E	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	F	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	G	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	H	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	I	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	J	153/156 (98%)	149 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	L	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
All	All	1836/1872 (98%)	1790 (98%)	46 (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	122/119 (102%)	121 (99%)	1 (1%)	81	70
1	B	122/119 (102%)	120 (98%)	2 (2%)	62	41
1	C	122/119 (102%)	122 (100%)	0	100	100
1	D	122/119 (102%)	121 (99%)	1 (1%)	81	70
1	E	122/119 (102%)	121 (99%)	1 (1%)	81	70
1	F	122/119 (102%)	121 (99%)	1 (1%)	81	70
1	G	122/119 (102%)	122 (100%)	0	100	100
1	H	122/119 (102%)	120 (98%)	2 (2%)	62	41
1	I	122/119 (102%)	122 (100%)	0	100	100
1	J	122/119 (102%)	119 (98%)	3 (2%)	47	22
1	K	122/119 (102%)	121 (99%)	1 (1%)	81	70
1	L	122/119 (102%)	121 (99%)	1 (1%)	81	70
All	All	1464/1428 (102%)	1451 (99%)	13 (1%)	78	65

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	80	PRO
1	J	2	ARG
1	L	2	ARG
1	J	11[B]	ILE

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Mol	Chain	Res	Type
1	K	2	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	6	ASN
1	K	24	GLN
1	L	6	ASN
1	E	106	HIS
1	E	95	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DHK	E	1162	-	12,12,12	5.47	10 (83%)	10,17,17	1.48	3 (30%)
3	DHK	F	1162	-	12,12,12	5.18	10 (83%)	10,17,17	2.20	5 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DHK	B	1162	-	12,12,12	4.86	10 (83%)	10,17,17	1.88	4 (40%)
3	DHK	C	1162	-	12,12,12	4.38	9 (75%)	10,17,17	1.86	3 (30%)
3	DHK	G	1162	-	12,12,12	4.68	10 (83%)	10,17,17	1.69	3 (30%)
3	DHK	J	1162	-	12,12,12	4.19	10 (83%)	10,17,17	2.14	3 (30%)
2	TRS	A	1152	-	7,7,7	1.08	1 (14%)	9,9,9	1.50	2 (22%)
3	DHK	K	1162	-	12,12,12	5.68	10 (83%)	10,17,17	2.18	5 (50%)
2	TRS	D	1152	-	7,7,7	1.34	2 (28%)	9,9,9	1.24	2 (22%)
2	TRS	G	1153	-	7,7,7	1.27	1 (14%)	9,9,9	1.39	1 (11%)
3	DHK	H	1162	-	12,12,12	4.59	10 (83%)	10,17,17	1.47	3 (30%)
3	DHK	I	1162	-	12,12,12	4.76	10 (83%)	10,17,17	1.64	2 (20%)
3	DHK	D	1162	-	12,12,12	6.05	9 (75%)	10,17,17	1.51	2 (20%)
3	DHK	L	1162	-	12,12,12	5.04	10 (83%)	10,17,17	1.70	2 (20%)
2	TRS	J	1152	-	7,7,7	1.02	0	9,9,9	1.15	0
3	DHK	A	1162	-	12,12,12	5.19	9 (75%)	10,17,17	1.72	3 (30%)

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	DHK	E	1162	-	-	0/4/20/20	0/1/1/1
3	DHK	F	1162	-	-	1/4/20/20	0/1/1/1
3	DHK	B	1162	-	-	0/4/20/20	0/1/1/1
3	DHK	C	1162	-	-	0/4/20/20	0/1/1/1
3	DHK	G	1162	-	-	0/4/20/20	0/1/1/1
3	DHK	J	1162	-	-	0/4/20/20	0/1/1/1
2	TRS	A	1152	-	-	0/9/9/9	-
3	DHK	K	1162	-	-	1/4/20/20	0/1/1/1
2	TRS	D	1152	-	-	0/9/9/9	-
2	TRS	G	1153	-	-	0/9/9/9	-
3	DHK	H	1162	-	-	1/4/20/20	0/1/1/1
3	DHK	I	1162	-	-	0/4/20/20	0/1/1/1
3	DHK	D	1162	-	-	1/4/20/20	0/1/1/1
3	DHK	L	1162	-	-	1/4/20/20	0/1/1/1
2	TRS	J	1152	-	-	0/9/9/9	-
3	DHK	A	1162	-	-	0/4/20/20	0/1/1/1

The worst 5 of 121 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1162	DHK	C5-C4	-13.84	1.39	1.52
3	K	1162	DHK	C5-C4	-11.66	1.41	1.52
3	F	1162	DHK	C5-C4	-10.70	1.42	1.52
3	E	1162	DHK	C5-C4	-10.41	1.42	1.52
3	C	1162	DHK	C5-C4	-10.27	1.42	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1162	DHK	C6-C1-C2	4.07	121.67	107.71
3	J	1162	DHK	O4-C4-C3	-3.89	100.34	110.90
3	K	1162	DHK	O5-C5-C4	3.85	116.21	109.73
3	F	1162	DHK	O4-C4-C5	3.35	115.98	110.28
3	F	1162	DHK	O3-C3-C2	-3.34	110.18	121.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1162	DHK	O1-C-C1-C6
3	K	1162	DHK	O1-C-C1-C6
3	F	1162	DHK	O1-C-C1-C2
3	H	1162	DHK	O1-C-C1-C2
3	L	1162	DHK	O1-C-C1-C2

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.