



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:19 PM GMT

PDB ID : 1GQO
Title : TYPE II DEHYDROQUINASE FROM BACILLUS SUBTILIS
Authors : Robinson, D.A.; Roszak, A.W.; Coggins, J.R.; Lapthorn, A.J.
Deposited on : 2001-11-28
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

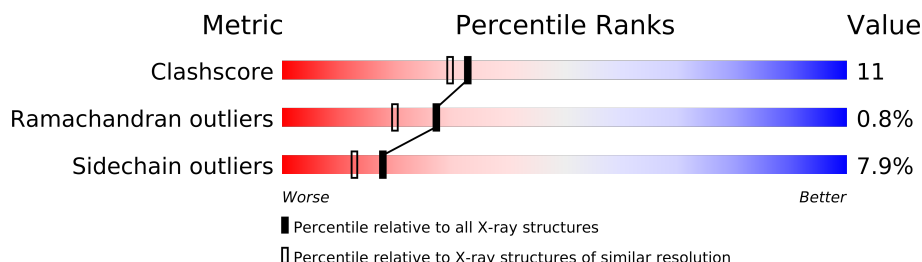
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	
1	B	143	
1	C	143	
1	D	143	
1	E	143	
1	F	143	
1	G	143	
1	H	143	
1	I	143	
1	J	143	
1	K	143	
1	L	143	
1	M	143	
1	N	143	
1	O	143	
1	P	143	
1	Q	143	

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Mol	Chain	Length	Quality of chain
1	R	143	
1	S	143	
1	T	143	
1	U	143	
1	V	143	
1	X	143	
1	Y	143	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28764 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DEHYDROQUINASE.

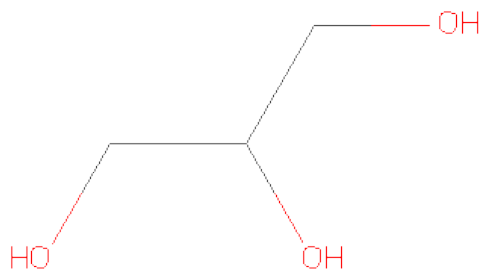
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	0	0	1
			1094	696	190	208			
1	B	143	Total	C	N	O	0	0	0
			1105	705	191	209			
1	C	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	D	142	Total	C	N	O	0	1	1
			1094	696	191	207			
1	E	142	Total	C	N	O	0	2	1
			1108	707	190	211			
1	F	142	Total	C	N	O	0	3	1
			1107	706	191	210			
1	G	142	Total	C	N	O	0	2	1
			1101	702	191	208			
1	H	142	Total	C	N	O	0	0	1
			1096	700	190	206			
1	I	142	Total	C	N	O	0	0	1
			1090	694	190	206			
1	J	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	K	137	Total	C	N	O	0	0	1
			1051	667	185	199			
1	L	142	Total	C	N	O	0	1	1
			1085	689	191	205			
1	M	142	Total	C	N	O	0	1	1
			1098	698	193	207			
1	N	133	Total	C	N	O	0	0	1
			1028	656	178	194			
1	O	142	Total	C	N	O	0	0	1
			1096	697	193	206			
1	P	142	Total	C	N	O	0	0	1
			1099	703	190	206			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	0	0	1
			1109	708	193	208			
1	R	142	Total	C	N	O	0	1	1
			1094	696	190	208			
1	S	142	Total	C	N	O	0	0	1
			1108	707	193	208			
1	T	142	Total	C	N	O	0	1	1
			1104	705	190	209			
1	U	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	V	136	Total	C	N	O	0	0	1
			1056	674	184	198			
1	X	134	Total	C	N	O	0	0	1
			1034	659	179	196			
1	Y	142	Total	C	N	O	0	0	1
			1096	700	190	206			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			5	3	2		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			5	3	2		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	J	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	M	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	N	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		
2	O	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	P	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	Q	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	R	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	S	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	T	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	U	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		
2	V	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	X	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		
2	X	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		
2	Y	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	98	Total	O	0	0
			98	98		
3	C	100	Total	O	0	0
			100	100		
3	D	96	Total	O	0	0
			96	96		
3	E	93	Total	O	0	0
			93	93		
3	F	91	Total	O	0	0
			91	91		
3	G	91	Total	O	0	0
			91	91		
3	H	75	Total	O	0	0
			75	75		
3	I	91	Total	O	0	0
			91	91		
3	J	91	Total	O	0	0
			91	91		
3	K	83	Total	O	0	0
			83	83		
3	L	86	Total	O	0	0
			86	86		
3	M	97	Total	O	0	0
			97	97		

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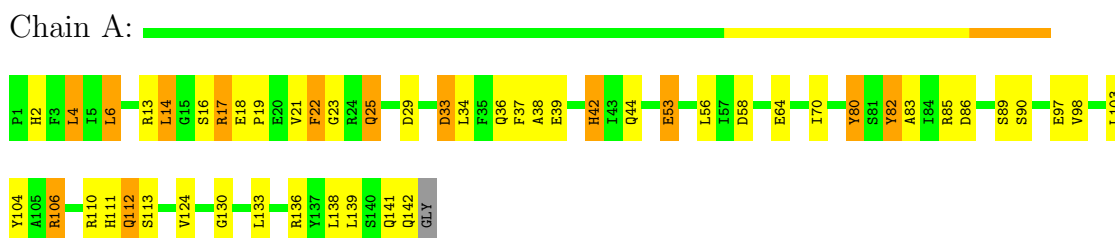
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	N	96	Total 96	O 96	0	0
3	O	89	Total 89	O 89	0	0
3	P	97	Total 97	O 97	0	0
3	Q	97	Total 97	O 97	0	0
3	R	103	Total 103	O 103	0	0
3	S	84	Total 84	O 84	0	0
3	T	87	Total 87	O 87	0	0
3	U	101	Total 101	O 101	0	0
3	V	107	Total 107	O 107	0	0
3	X	79	Total 79	O 79	0	0
3	Y	80	Total 80	O 80	0	0

3 Residue-property plots

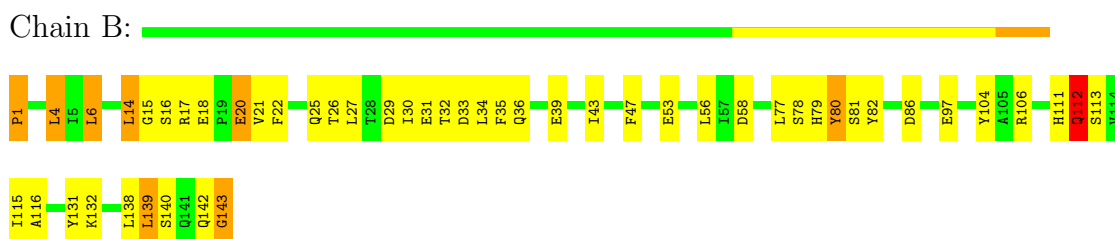
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

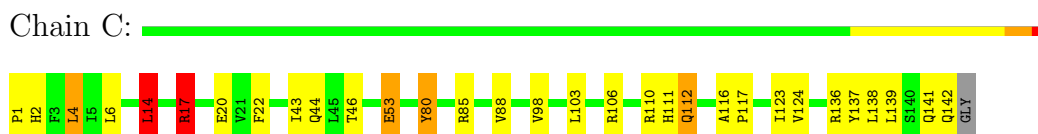
• Molecule 1: DEHYDROQUINASE



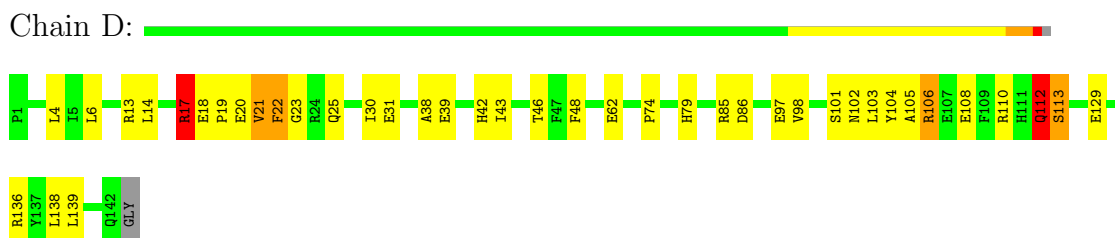
• Molecule 1: DEHYDROQUINASE



• Molecule 1: DEHYDROQUINASE

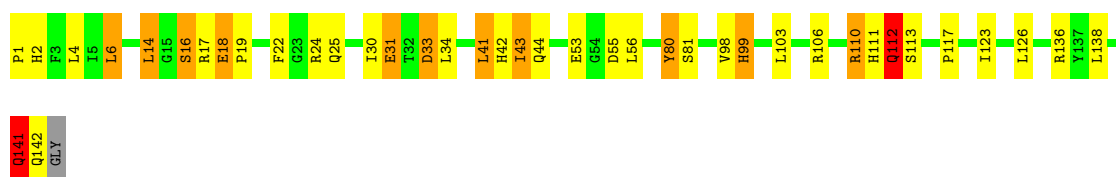


• Molecule 1: DEHYDROQUINASE



• Molecule 1: DEHYDROQUINASE





- Molecule 1: DEHYDROQUINASE

Chain F:

- Molecule 1: DEHYDROQUINASE

Chain G:

- Molecule 1: DEHYDROQUINASE

Chain H:

- Molecule 1: DEHYDROQUINASE

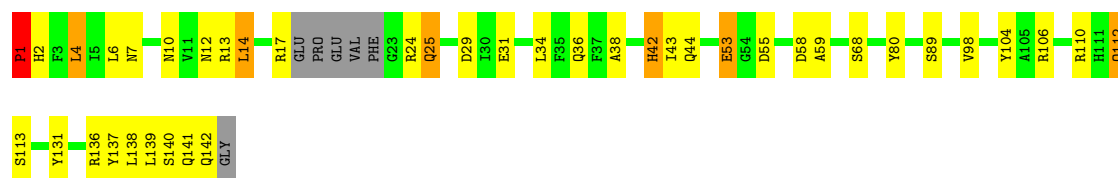
Chain I:

- Molecule 1: DEHYDROQUINASE

Chain J:

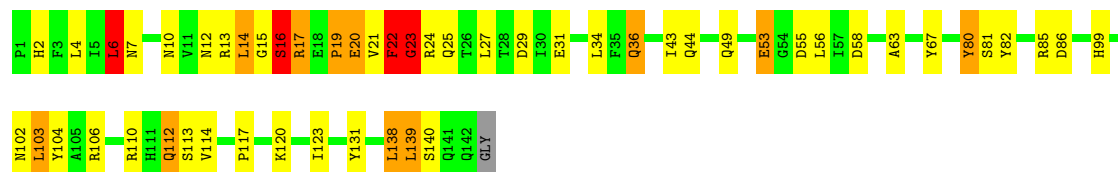
- Molecule 1: DEHYDROQUINASE

Chain K: 



- Molecule 1: DEHYDROQUINASE

Chain L: 



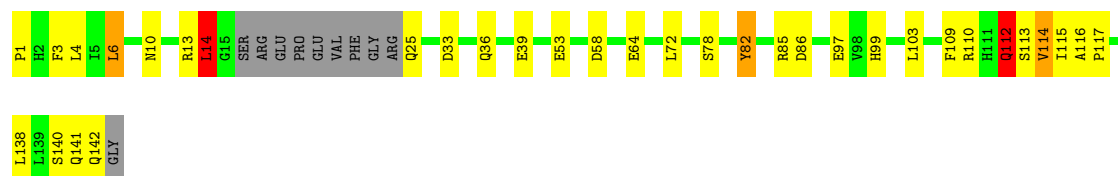
- Molecule 1: DEHYDROQUINASE

Chain M: 



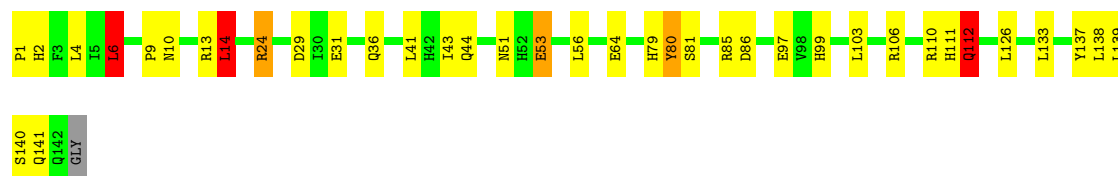
- Molecule 1: DEHYDROQUINASE

Chain N: 



- Molecule 1: DEHYDROQUINASE

Chain O: 



- Molecule 1: DEHYDROQUINASE

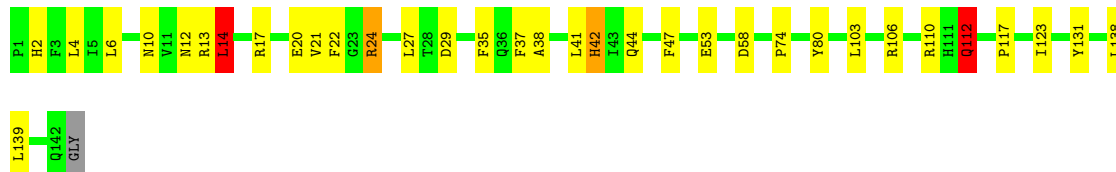
Chain P: 





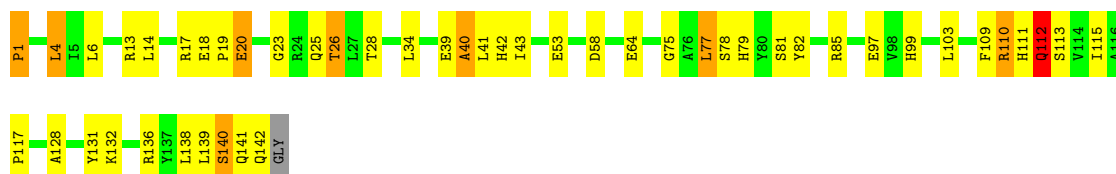
• Molecule 1: DEHYDROQUINASE

Chain Q:



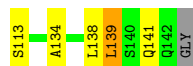
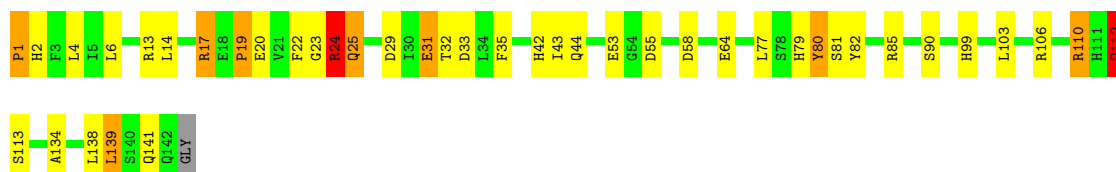
• Molecule 1: DEHYDROQUINASE

Chain R:



• Molecule 1: DEHYDROQUINASE

Chain S:



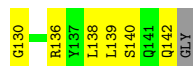
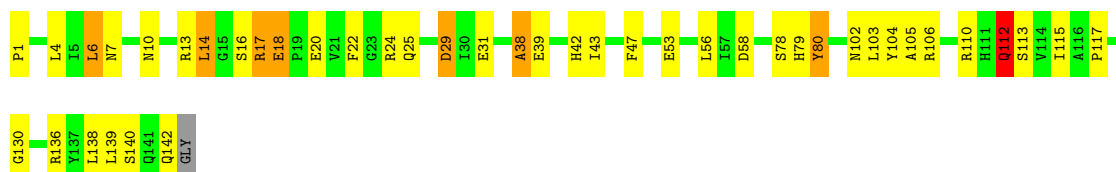
• Molecule 1: DEHYDROQUINASE

Chain T:



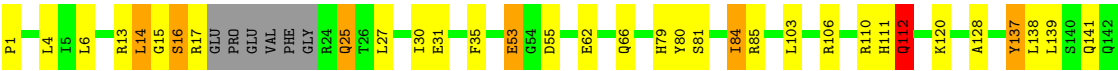
• Molecule 1: DEHYDROQUINASE

Chain U:



• Molecule 1: DEHYDROQUINASE

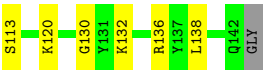
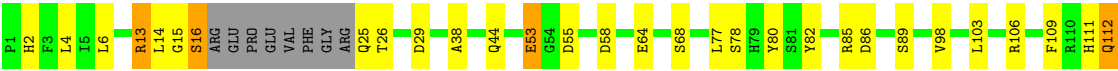
Chain V:



GLY

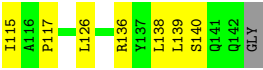
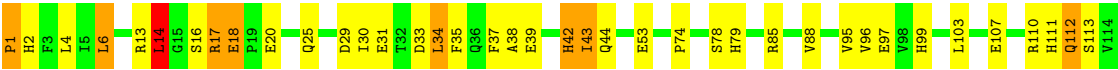
• Molecule 1: DEHYDROQUINASE

Chain X:



• Molecule 1: DEHYDROQUINASE

Chain Y:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.21Å 195.61Å 97.36Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	21.84 – 2.10	Depositor
% Data completeness (in resolution range)	86.0 (21.84-2.10)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28764	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.91	0/1117	1.81	27/1519 (1.8%)
1	B	2.48	2/1128 (0.2%)	1.63	16/1529 (1.0%)
1	C	0.92	0/1116	1.63	13/1518 (0.9%)
1	D	0.93	0/1122	1.78	16/1526 (1.0%)
1	E	1.14	1/1143 (0.1%)	2.27	29/1554 (1.9%)
1	F	0.89	1/1146 (0.1%)	1.64	14/1558 (0.9%)
1	G	0.87	0/1135	1.64	16/1543 (1.0%)
1	H	1.14	1/1121 (0.1%)	2.09	28/1525 (1.8%)
1	I	1.02	1/1113 (0.1%)	1.81	29/1514 (1.9%)
1	J	0.88	0/1116	1.68	18/1518 (1.2%)
1	K	0.96	0/1071	1.79	28/1454 (1.9%)
1	L	0.97	0/1112	1.96	41/1513 (2.7%)
1	M	0.94	1/1126 (0.1%)	1.79	18/1530 (1.2%)
1	N	0.94	0/1048	1.89	22/1424 (1.5%)
1	O	0.88	0/1119	1.75	23/1521 (1.5%)
1	P	0.94	1/1123 (0.1%)	1.74	21/1527 (1.4%)
1	Q	0.93	0/1133	1.87	22/1539 (1.4%)
1	R	0.91	0/1122	1.80	27/1526 (1.8%)
1	S	0.91	0/1132	1.75	22/1538 (1.4%)
1	T	0.89	0/1133	1.71	23/1540 (1.5%)
1	U	0.95	0/1116	1.72	11/1518 (0.7%)
1	V	0.88	0/1077	1.62	18/1462 (1.2%)
1	X	0.94	1/1054 (0.1%)	1.84	24/1432 (1.7%)
1	Y	0.94	1/1120 (0.1%)	1.75	17/1523 (1.1%)
All	All	1.06	10/26743 (0.0%)	1.80	523/36351 (1.4%)

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	E	0	1
1	H	0	1
1	I	0	1
1	K	0	1
1	R	0	1
1	X	0	1
All	All	0	6

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	GLY	C-OXT	76.84	2.69	1.23
1	H	141	GLN	C-N	23.02	1.86	1.34
1	E	141	GLN	C-N	-21.85	0.83	1.34
1	B	39	GLU	CB-CG	-5.93	1.40	1.52
1	F	39	GLU	CB-CG	-5.50	1.41	1.52

The worst 5 of 523 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	141	GLN	O-C-N	-53.94	36.39	122.70
1	H	141	GLN	O-C-N	-27.34	78.96	122.70
1	H	141	GLN	CA-C-N	-26.95	57.92	117.20
1	Q	24	ARG	CD-NE-CZ	18.41	149.38	123.60
1	N	82	TYR	CB-CG-CD2	17.36	131.42	121.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	141	GLN	Mainchain
1	H	40	ALA	Mainchain
1	I	115	ILE	Mainchain
1	K	12	ASN	Mainchain
1	R	111	HIS	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1094	0	1059	31	0
1	B	1105	0	1065	27	0
1	C	1093	0	1064	23	0
1	D	1094	0	1059	22	0
1	E	1108	0	1078	24	0
1	F	1107	0	1076	18	0
1	G	1101	0	1067	21	0
1	H	1096	0	1061	31	0
1	I	1090	0	1055	32	0
1	J	1093	0	1064	23	0
1	K	1051	0	1021	17	0
1	L	1085	0	1050	26	0
1	M	1098	0	1069	24	0
1	N	1028	0	1006	15	0
1	O	1096	0	1066	24	0
1	P	1099	0	1071	25	0
1	Q	1109	0	1086	18	0
1	R	1094	0	1055	23	0
1	S	1108	0	1084	25	0
1	T	1104	0	1076	16	0
1	U	1093	0	1064	35	0
1	V	1056	0	1034	21	0
1	X	1034	0	1012	17	0
1	Y	1096	0	1062	28	0
2	A	18	0	24	5	0
2	B	18	0	24	5	0
2	C	18	0	24	7	0
2	D	18	0	23	5	0
2	E	17	0	21	3	0
2	F	17	0	20	3	0
2	G	18	0	24	6	0
2	H	18	0	24	5	0
2	I	18	0	24	4	0
2	J	18	0	24	2	0
2	K	18	0	24	6	0
2	L	18	0	23	7	0
2	M	18	0	24	3	0
2	N	18	0	23	3	0
2	O	18	0	24	8	0
2	P	18	0	24	6	0
2	Q	18	0	24	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	R	18	0	24	6	0
2	S	18	0	24	9	0
2	T	18	0	24	4	0
2	U	18	0	24	10	0
2	V	18	0	24	5	0
2	X	18	0	23	3	0
2	Y	18	0	24	7	0
3	A	90	0	0	14	0
3	B	98	0	0	10	0
3	C	100	0	0	12	0
3	D	96	0	0	6	0
3	E	93	0	0	9	0
3	F	91	0	0	8	0
3	G	91	0	0	9	0
3	H	75	0	0	12	0
3	I	91	0	0	8	0
3	J	91	0	0	10	0
3	K	83	0	0	2	0
3	L	86	0	0	8	0
3	M	97	0	0	8	0
3	N	96	0	0	7	0
3	O	89	0	0	9	0
3	P	97	0	0	10	0
3	Q	97	0	0	9	0
3	R	103	0	0	13	0
3	S	84	0	0	10	0
3	T	87	0	0	8	0
3	U	101	0	0	13	0
3	V	107	0	0	9	0
3	X	79	0	0	10	0
3	Y	80	0	0	12	0
All	All	28764	0	25969	589	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 589 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:N:141:GLN:HA	1:N:142:GLN:N	1.42	1.23
1:F:142:GLN:N	3:F:2084:HOH:O	1.69	1.20
1:U:140:SER:O	1:U:142:GLN:N	1.81	1.13
1:U:117:PRO:HG3	2:U:151:GOL:H11	1.36	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:14:LEU:HD13	2:M:152:GOL:H11	1.38	1.04

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	139/143 (97%)	131 (94%)	8 (6%)	0	100	100
1	B	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	30	23
1	C	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	D	140/143 (98%)	132 (94%)	7 (5%)	1 (1%)	30	23
1	E	142/143 (99%)	130 (92%)	10 (7%)	2 (1%)	16	9
1	F	142/143 (99%)	133 (94%)	7 (5%)	2 (1%)	16	9
1	G	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	16	9
1	H	140/143 (98%)	132 (94%)	8 (6%)	0	100	100
1	I	139/143 (97%)	130 (94%)	5 (4%)	4 (3%)	7	2
1	J	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	K	132/143 (92%)	127 (96%)	5 (4%)	0	100	100
1	L	140/143 (98%)	128 (91%)	6 (4%)	6 (4%)	4	1
1	M	140/143 (98%)	133 (95%)	5 (4%)	2 (1%)	16	9
1	N	128/143 (90%)	124 (97%)	4 (3%)	0	100	100
1	O	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	P	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	16	9
1	Q	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	R	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	30	23
1	S	139/143 (97%)	132 (95%)	7 (5%)	0	100	100
1	T	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	30	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	16	9
1	V	131/143 (92%)	125 (95%)	5 (4%)	1 (1%)	27	20
1	X	129/143 (90%)	122 (95%)	7 (5%)	0	100	100
1	Y	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	30	23
All	All	3314/3432 (97%)	3130 (94%)	156 (5%)	28 (1%)	27	20

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	16	SER
1	L	22	PHE
1	L	23	GLY
1	P	16	SER
1	V	16	SER

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	115/120 (96%)	105 (91%)	10 (9%)	15	10
1	B	115/120 (96%)	106 (92%)	9 (8%)	18	13
1	C	115/120 (96%)	108 (94%)	7 (6%)	26	22
1	D	115/120 (96%)	102 (89%)	13 (11%)	9	4
1	E	119/120 (99%)	110 (92%)	9 (8%)	19	14
1	F	119/120 (99%)	112 (94%)	7 (6%)	28	23
1	G	117/120 (98%)	108 (92%)	9 (8%)	18	13
1	H	115/120 (96%)	102 (89%)	13 (11%)	9	4
1	I	114/120 (95%)	105 (92%)	9 (8%)	18	13
1	J	115/120 (96%)	107 (93%)	8 (7%)	21	17
1	K	110/120 (92%)	101 (92%)	9 (8%)	17	11
1	L	113/120 (94%)	104 (92%)	9 (8%)	17	12
1	M	116/120 (97%)	107 (92%)	9 (8%)	18	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	109/120 (91%)	102 (94%)	7 (6%)	25	20
1	O	115/120 (96%)	108 (94%)	7 (6%)	26	22
1	P	116/120 (97%)	105 (90%)	11 (10%)	12	8
1	Q	118/120 (98%)	110 (93%)	8 (7%)	22	18
1	R	115/120 (96%)	105 (91%)	10 (9%)	15	10
1	S	118/120 (98%)	105 (89%)	13 (11%)	9	5
1	T	118/120 (98%)	108 (92%)	10 (8%)	15	10
1	U	115/120 (96%)	108 (94%)	7 (6%)	26	22
1	V	112/120 (93%)	105 (94%)	7 (6%)	25	21
1	X	110/120 (92%)	103 (94%)	7 (6%)	25	20
1	Y	115/120 (96%)	100 (87%)	15 (13%)	6	3
All	All	2759/2880 (96%)	2536 (92%)	223 (8%)	18	12

5 of 223 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	42	HIS
1	N	25	GLN
1	X	112	GLN
1	L	4	LEU
1	M	6	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	141	GLN
1	M	66	GLN
1	V	25	GLN
1	L	66	GLN
1	O	66	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

72 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	$\# Z > 2$
2	GOL	A	150	-	5,5,5	0.87	0	5,5,5	0.52	0
2	GOL	A	151	-	5,5,5	0.61	0	5,5,5	1.99	2 (40%)
2	GOL	A	152	-	5,5,5	0.69	0	5,5,5	1.02	0
2	GOL	B	150	-	5,5,5	0.77	0	5,5,5	1.12	0
2	GOL	B	151	-	5,5,5	0.79	0	5,5,5	1.17	1 (20%)
2	GOL	B	152	-	5,5,5	0.54	0	5,5,5	0.50	0
2	GOL	C	150	-	5,5,5	1.00	0	5,5,5	1.08	1 (20%)
2	GOL	C	151	-	5,5,5	0.71	0	5,5,5	0.98	0
2	GOL	C	152	-	5,5,5	0.75	0	5,5,5	0.76	0
2	GOL	D	150	-	5,5,5	0.99	0	5,5,5	2.16	2 (40%)
2	GOL	D	151	-	5,5,5	0.79	0	5,5,5	0.80	0
2	GOL	D	152	-	5,5,5	0.51	0	5,5,5	1.96	3 (60%)
2	GOL	E	150	-	5,5,5	0.95	0	5,5,5	0.79	0
2	GOL	E	151	-	5,5,5	0.55	0	5,5,5	0.83	0
2	GOL	E	152	-	3,4,5	0.92	0	2,4,5	3.41	1 (50%)
2	GOL	F	150	-	5,5,5	1.15	0	5,5,5	1.74	2 (40%)
2	GOL	F	151	-	5,5,5	0.48	0	5,5,5	0.82	0
2	GOL	F	152	-	3,4,5	1.07	0	2,4,5	2.40	1 (50%)
2	GOL	G	150	-	5,5,5	0.55	0	5,5,5	1.22	1 (20%)
2	GOL	G	151	-	5,5,5	0.57	0	5,5,5	1.46	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	G	152	-	5,5,5	0.65	0	5,5,5	1.91	2 (40%)
2	GOL	H	150	-	5,5,5	0.87	0	5,5,5	1.47	1 (20%)
2	GOL	H	151	-	5,5,5	0.65	0	5,5,5	0.77	0
2	GOL	H	152	-	5,5,5	0.74	0	5,5,5	1.16	0
2	GOL	I	150	-	5,5,5	0.74	0	5,5,5	1.64	2 (40%)
2	GOL	I	151	-	5,5,5	0.56	0	5,5,5	0.98	0
2	GOL	I	152	-	5,5,5	0.49	0	5,5,5	1.00	0
2	GOL	J	150	-	5,5,5	0.91	0	5,5,5	2.11	2 (40%)
2	GOL	J	151	-	5,5,5	0.62	0	5,5,5	1.29	1 (20%)
2	GOL	J	152	-	5,5,5	0.72	0	5,5,5	1.09	1 (20%)
2	GOL	K	150	-	5,5,5	1.03	1 (20%)	5,5,5	1.20	0
2	GOL	K	151	-	5,5,5	0.62	0	5,5,5	0.66	0
2	GOL	K	152	-	5,5,5	0.75	0	5,5,5	1.05	0
2	GOL	L	150	-	5,5,5	0.95	0	5,5,5	2.16	2 (40%)
2	GOL	L	151	-	5,5,5	0.52	0	5,5,5	0.92	0
2	GOL	L	152	-	5,5,5	0.47	0	5,5,5	1.19	0
2	GOL	M	150	-	5,5,5	0.98	0	5,5,5	1.19	0
2	GOL	M	151	-	5,5,5	0.54	0	5,5,5	0.96	0
2	GOL	M	152	-	5,5,5	0.49	0	5,5,5	1.05	0
2	GOL	N	150	-	5,5,5	1.08	0	5,5,5	1.46	1 (20%)
2	GOL	N	151	-	5,5,5	0.68	0	5,5,5	1.48	1 (20%)
2	GOL	N	152	-	5,5,5	0.58	0	5,5,5	0.96	0
2	GOL	O	150	-	5,5,5	1.14	0	5,5,5	1.58	1 (20%)
2	GOL	O	151	-	5,5,5	0.72	0	5,5,5	1.02	1 (20%)
2	GOL	O	152	-	5,5,5	0.68	0	5,5,5	0.50	0
2	GOL	P	150	-	5,5,5	1.07	1 (20%)	5,5,5	1.10	0
2	GOL	P	151	-	5,5,5	0.69	0	5,5,5	0.72	0
2	GOL	P	152	-	5,5,5	0.60	0	5,5,5	0.76	0
2	GOL	Q	150	-	5,5,5	1.10	0	5,5,5	1.43	1 (20%)
2	GOL	Q	151	-	5,5,5	0.68	0	5,5,5	0.53	0
2	GOL	Q	152	-	5,5,5	0.84	0	5,5,5	0.77	0
2	GOL	R	150	-	5,5,5	1.70	2 (40%)	5,5,5	2.11	3 (60%)
2	GOL	R	151	-	5,5,5	0.39	0	5,5,5	1.47	1 (20%)
2	GOL	R	152	-	5,5,5	0.57	0	5,5,5	0.85	0
2	GOL	S	150	-	5,5,5	1.76	1 (20%)	5,5,5	1.38	1 (20%)
2	GOL	S	151	-	5,5,5	0.72	0	5,5,5	1.77	2 (40%)
2	GOL	S	152	-	5,5,5	0.50	0	5,5,5	1.04	0
2	GOL	T	150	-	5,5,5	0.95	0	5,5,5	1.63	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	T	151	-	5,5,5	0.54	0	5,5,5	0.57	0
2	GOL	T	152	-	5,5,5	0.61	0	5,5,5	0.55	0
2	GOL	U	150	-	5,5,5	0.90	0	5,5,5	1.44	1 (20%)
2	GOL	U	151	-	5,5,5	0.33	0	5,5,5	0.71	0
2	GOL	U	152	-	5,5,5	0.67	0	5,5,5	0.55	0
2	GOL	V	150	-	5,5,5	0.51	0	5,5,5	1.16	1 (20%)
2	GOL	V	151	-	5,5,5	0.69	0	5,5,5	1.95	1 (20%)
2	GOL	V	152	-	5,5,5	0.68	0	5,5,5	1.22	0
2	GOL	X	150	-	5,5,5	1.30	1 (20%)	5,5,5	0.89	0
2	GOL	X	151	-	5,5,5	0.73	0	5,5,5	1.58	1 (20%)
2	GOL	X	152	-	5,5,5	0.73	0	5,5,5	0.46	0
2	GOL	Y	150	-	5,5,5	0.69	0	5,5,5	1.67	2 (40%)
2	GOL	Y	151	-	5,5,5	0.49	0	5,5,5	0.96	0
2	GOL	Y	152	-	5,5,5	0.88	0	5,5,5	0.64	0

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	GOL	A	150	-	-	0/4/4/4	0/0/0/0
2	GOL	A	151	-	-	0/4/4/4	0/0/0/0
2	GOL	A	152	-	-	0/4/4/4	0/0/0/0
2	GOL	B	150	-	-	0/4/4/4	0/0/0/0
2	GOL	B	151	-	-	0/4/4/4	0/0/0/0
2	GOL	B	152	-	-	0/4/4/4	0/0/0/0
2	GOL	C	150	-	-	0/4/4/4	0/0/0/0
2	GOL	C	151	-	-	0/4/4/4	0/0/0/0
2	GOL	C	152	-	-	0/4/4/4	0/0/0/0
2	GOL	D	150	-	-	0/4/4/4	0/0/0/0
2	GOL	D	151	-	-	0/4/4/4	0/0/0/0
2	GOL	D	152	-	-	0/4/4/4	0/0/0/0
2	GOL	E	150	-	-	0/4/4/4	0/0/0/0
2	GOL	E	151	-	-	0/4/4/4	0/0/0/0
2	GOL	E	152	-	-	0/2/2/4	0/0/0/0
2	GOL	F	150	-	-	0/4/4/4	0/0/0/0
2	GOL	F	151	-	-	0/4/4/4	0/0/0/0
2	GOL	F	152	-	-	0/2/2/4	0/0/0/0
2	GOL	G	150	-	-	0/4/4/4	0/0/0/0
2	GOL	G	151	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	G	152	-	-	0/4/4/4	0/0/0/0
2	GOL	H	150	-	-	0/4/4/4	0/0/0/0
2	GOL	H	151	-	-	0/4/4/4	0/0/0/0
2	GOL	H	152	-	-	0/4/4/4	0/0/0/0
2	GOL	I	150	-	-	0/4/4/4	0/0/0/0
2	GOL	I	151	-	-	0/4/4/4	0/0/0/0
2	GOL	I	152	-	-	0/4/4/4	0/0/0/0
2	GOL	J	150	-	-	0/4/4/4	0/0/0/0
2	GOL	J	151	-	-	0/4/4/4	0/0/0/0
2	GOL	J	152	-	-	0/4/4/4	0/0/0/0
2	GOL	K	150	-	-	0/4/4/4	0/0/0/0
2	GOL	K	151	-	-	0/4/4/4	0/0/0/0
2	GOL	K	152	-	-	0/4/4/4	0/0/0/0
2	GOL	L	150	-	-	0/4/4/4	0/0/0/0
2	GOL	L	151	-	-	0/4/4/4	0/0/0/0
2	GOL	L	152	-	-	0/4/4/4	0/0/0/0
2	GOL	M	150	-	-	0/4/4/4	0/0/0/0
2	GOL	M	151	-	-	0/4/4/4	0/0/0/0
2	GOL	M	152	-	-	0/4/4/4	0/0/0/0
2	GOL	N	150	-	-	0/4/4/4	0/0/0/0
2	GOL	N	151	-	-	0/4/4/4	0/0/0/0
2	GOL	N	152	-	-	0/4/4/4	0/0/0/0
2	GOL	O	150	-	-	0/4/4/4	0/0/0/0
2	GOL	O	151	-	-	0/4/4/4	0/0/0/0
2	GOL	O	152	-	-	0/4/4/4	0/0/0/0
2	GOL	P	150	-	-	0/4/4/4	0/0/0/0
2	GOL	P	151	-	-	0/4/4/4	0/0/0/0
2	GOL	P	152	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	150	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	151	-	-	0/4/4/4	0/0/0/0
2	GOL	Q	152	-	-	0/4/4/4	0/0/0/0
2	GOL	R	150	-	-	0/4/4/4	0/0/0/0
2	GOL	R	151	-	-	0/4/4/4	0/0/0/0
2	GOL	R	152	-	-	0/4/4/4	0/0/0/0
2	GOL	S	150	-	-	0/4/4/4	0/0/0/0
2	GOL	S	151	-	-	0/4/4/4	0/0/0/0
2	GOL	S	152	-	-	0/4/4/4	0/0/0/0
2	GOL	T	150	-	-	0/4/4/4	0/0/0/0
2	GOL	T	151	-	-	0/4/4/4	0/0/0/0
2	GOL	T	152	-	-	0/4/4/4	0/0/0/0
2	GOL	U	150	-	-	0/4/4/4	0/0/0/0
2	GOL	U	151	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	U	152	-	-	0/4/4/4	0/0/0/0
2	GOL	V	150	-	-	0/4/4/4	0/0/0/0
2	GOL	V	151	-	-	0/4/4/4	0/0/0/0
2	GOL	V	152	-	-	0/4/4/4	0/0/0/0
2	GOL	X	150	-	-	0/4/4/4	0/0/0/0
2	GOL	X	151	-	-	0/4/4/4	0/0/0/0
2	GOL	X	152	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	150	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	151	-	-	0/4/4/4	0/0/0/0
2	GOL	Y	152	-	-	0/4/4/4	0/0/0/0

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	150	GOL	O1-C1	3.55	1.57	1.42
2	X	150	GOL	O1-C1	2.64	1.53	1.42
2	R	150	GOL	C1-C2	2.40	1.62	1.52
2	K	150	GOL	O1-C1	2.06	1.51	1.42
2	R	150	GOL	O1-C1	2.05	1.51	1.42

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	152	GOL	O2-C2-C1	4.80	117.35	109.15
2	V	151	GOL	O2-C2-C1	3.84	125.71	108.22
2	J	150	GOL	C3-C2-C1	3.71	127.66	111.26
2	A	151	GOL	O2-C2-C1	3.39	123.68	108.22
2	F	152	GOL	O2-C2-C1	3.33	114.85	109.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.