wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 08:21 AM EDT

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 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 (i) 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 (i)) were used in the production of this report:

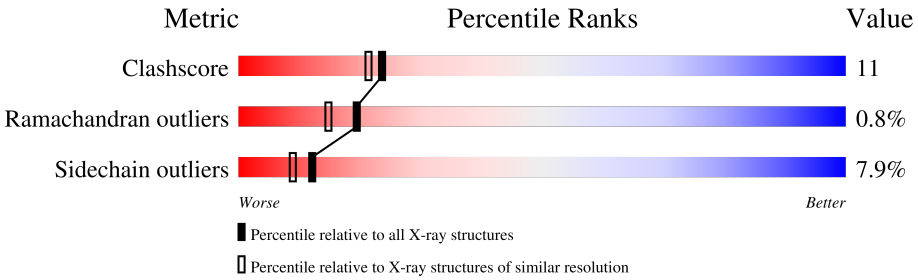
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	143	64% 27% 9% •
1	B	143	65% 29% 6% •
1	C	143	78% 17% • ••
1	D	143	71% 24% • ••
1	E	143	71% 19% 8% ••
1	F	143	78% 19% •••
1	G	143	71% 24% • ••
1	H	143	63% 29% 5% ••

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Mol	Chain	Length	Quality of chain
1	I	143	62% 27% 8%
1	J	143	69% 26% 5%
1	K	143	67% 24%
1	L	143	62% 27% 8%
1	M	143	69% 27%
1	N	143	69% 20% 7%
1	O	143	73% 22%
1	P	143	69% 23% 6%
1	Q	143	76% 21%
1	R	143	66% 27% 6%
1	S	143	70% 22% 6%
1	T	143	76% 17% 6%
1	U	143	69% 24% 5%
1	V	143	72% 18% 5%
1	X	143	69% 22% 6%
1	Y	143	67% 26% 6%

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
2	GOL	C	151	-	-	X	-
2	GOL	D	151	-	-	X	-
2	GOL	D	152	-	X	-	-
2	GOL	F	150	-	X	-	-
2	GOL	G	151	-	-	X	-
2	GOL	I	150	-	X	-	-
2	GOL	K	152	-	-	X	-
2	GOL	L	150	-	X	-	-
2	GOL	L	151	-	-	X	-
2	GOL	O	150	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	O	151	-	-	X	-
2	GOL	O	152	-	-	X	-
2	GOL	P	151	-	-	X	-
2	GOL	Q	151	-	-	X	-
2	GOL	R	150	-	X	-	-
2	GOL	R	151	-	-	X	-
2	GOL	S	150	-	X	-	-
2	GOL	S	151	-	-	X	-
2	GOL	S	152	-	-	X	-
2	GOL	U	151	-	-	X	-
2	GOL	Y	151	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 28764 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 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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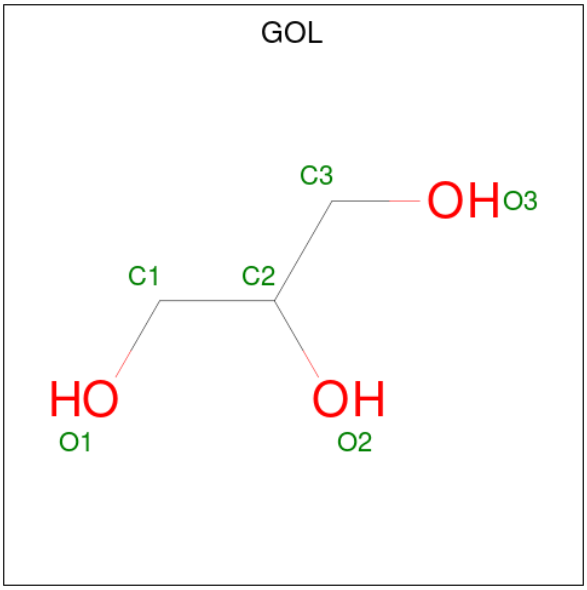
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	Q	142	Total	C	N	O	0	0	1
			1109	708	193	208			
1	R	142	Total	C	N	O	0	1	1
			1094	696	190	208			
1	S	142	Total	C	N	O	0	0	1
			1108	707	193	208			
1	T	142	Total	C	N	O	0	1	1
			1104	705	190	209			
1	U	142	Total	C	N	O	0	0	1
			1093	697	190	206			
1	V	136	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 6 3 3	0	0
2	P	1	Total C O 6 3 3	0	0
2	P	1	Total C O 6 3 3	0	0
2	Q	1	Total C O 6 3 3	0	0
2	Q	1	Total C O 6 3 3	0	0
2	Q	1	Total C O 6 3 3	0	0
2	R	1	Total C O 6 3 3	0	0
2	R	1	Total C O 6 3 3	0	0
2	R	1	Total C O 6 3 3	0	0
2	S	1	Total C O 6 3 3	0	0
2	S	1	Total C O 6 3 3	0	0
2	S	1	Total C O 6 3 3	0	0
2	T	1	Total C O 6 3 3	0	0
2	T	1	Total C O 6 3 3	0	0
2	T	1	Total C O 6 3 3	0	0
2	U	1	Total C O 6 3 3	0	0
2	U	1	Total C O 6 3 3	0	0
2	U	1	Total C O 6 3 3	0	0
2	V	1	Total C O 6 3 3	0	0
2	V	1	Total C O 6 3 3	0	0
2	V	1	Total C O 6 3 3	0	0

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

- Molecule 3 is water.

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

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

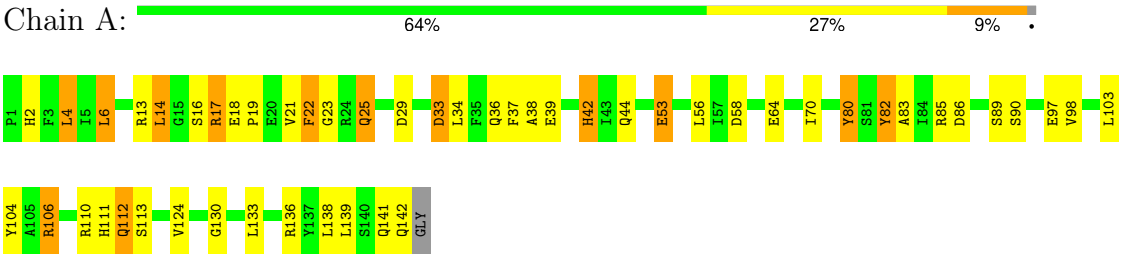
3 Residue-property plots (i)

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.

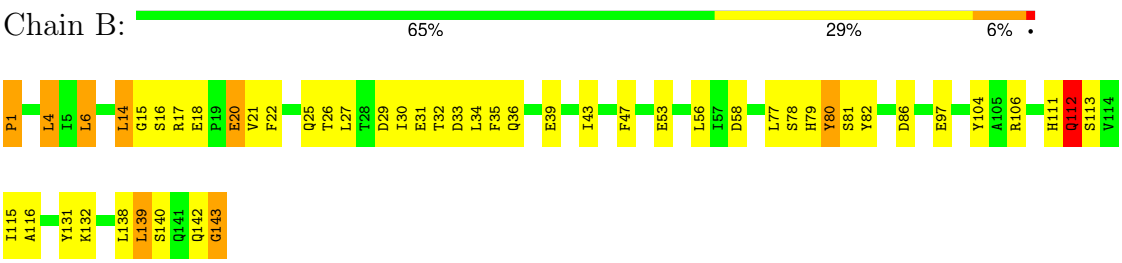
• Molecule 1: DEHYDROQUINASE

Chain A:



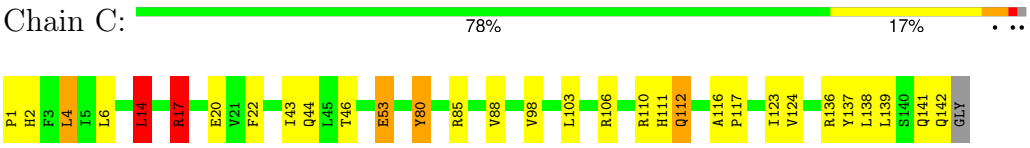
• Molecule 1: DEHYDROQUINASE

Chain B:



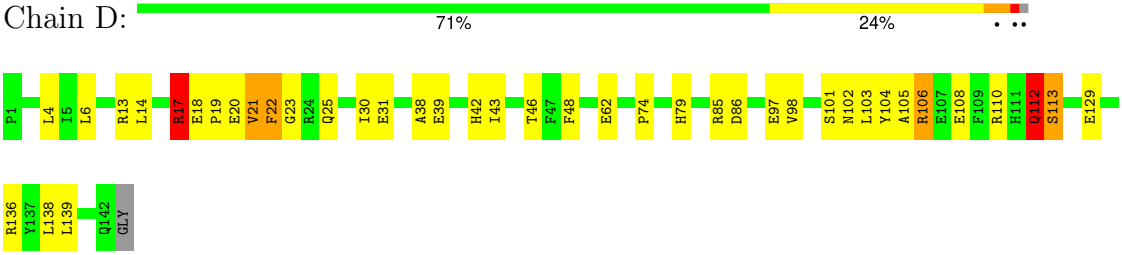
• Molecule 1: DEHYDROQUINASE

Chain C:



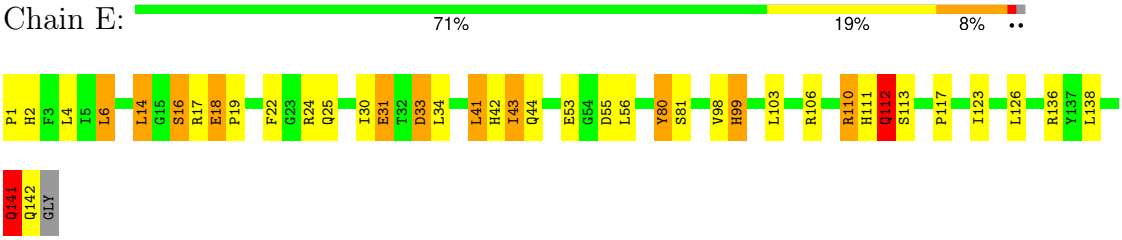
• Molecule 1: DEHYDROQUINASE

Chain D:



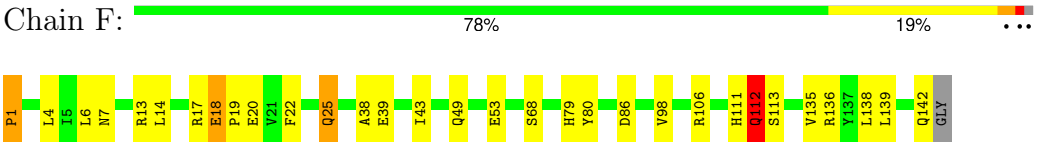
• Molecule 1: DEHYDROQUINASE

Chain E:



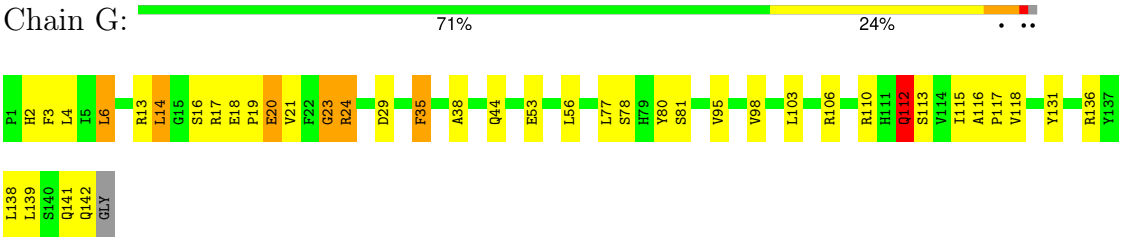
• Molecule 1: DEHYDROQUINASE

Chain F:



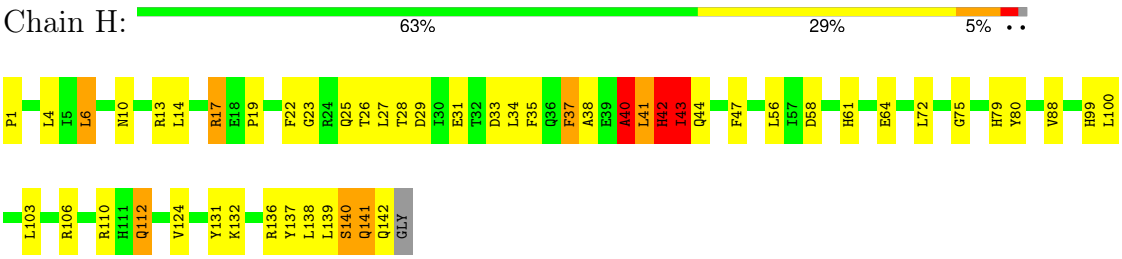
• Molecule 1: DEHYDROQUINASE

Chain G:



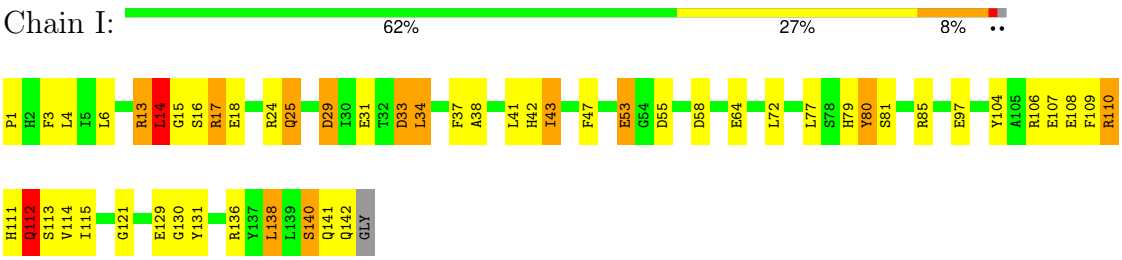
• Molecule 1: DEHYDROQUINASE

Chain H:



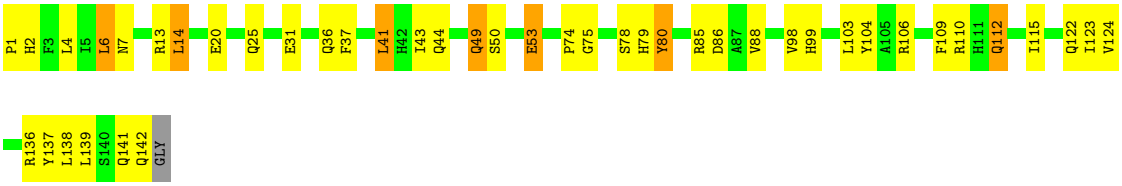
• Molecule 1: DEHYDROQUINASE

Chain I:



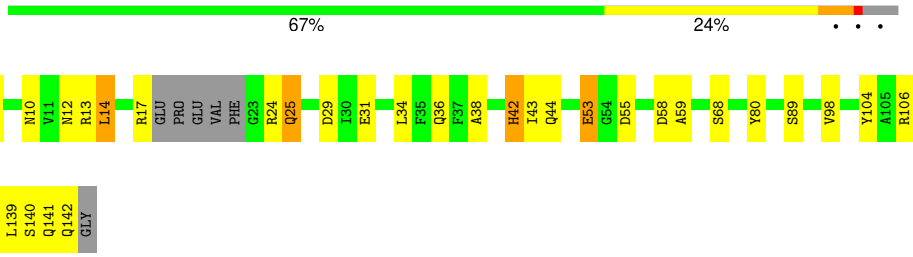
• Molecule 1: DEHYDROQUINASE

Chain J:



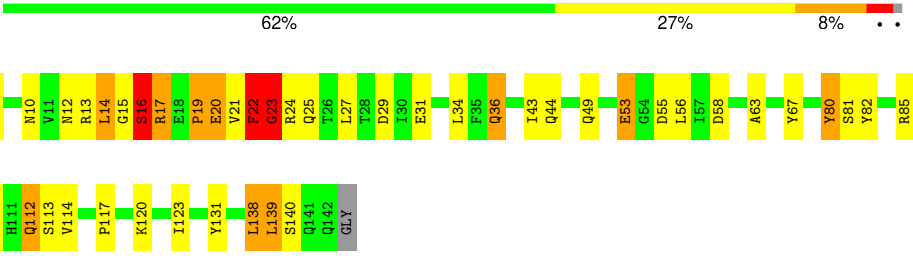
• Molecule 1: DEHYDROQUINASE

Chain K:



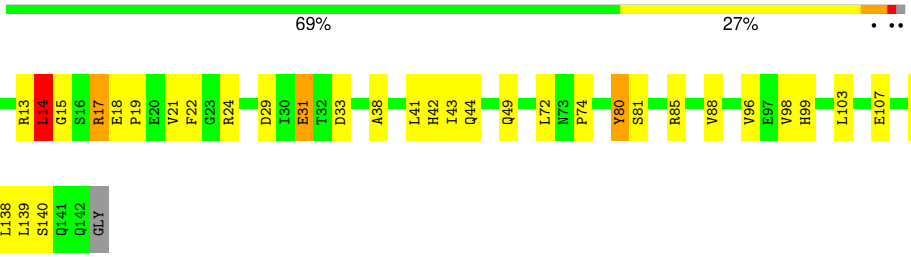
• Molecule 1: DEHYDROQUINASE

Chain L:



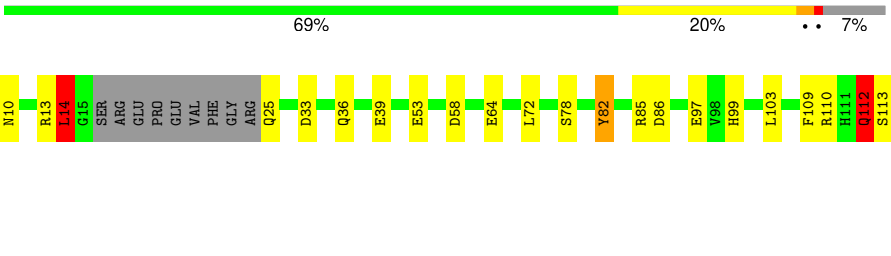
• Molecule 1: DEHYDROQUINASE

Chain M:



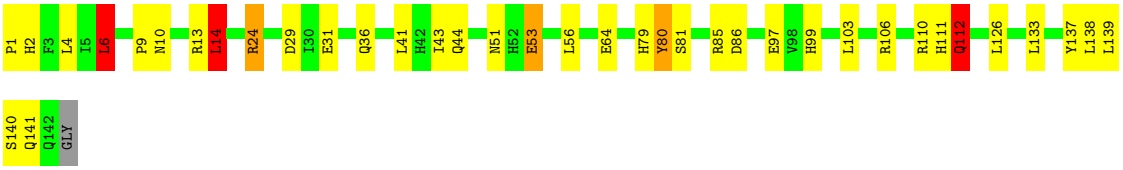
• Molecule 1: DEHYDROQUINASE

Chain N:



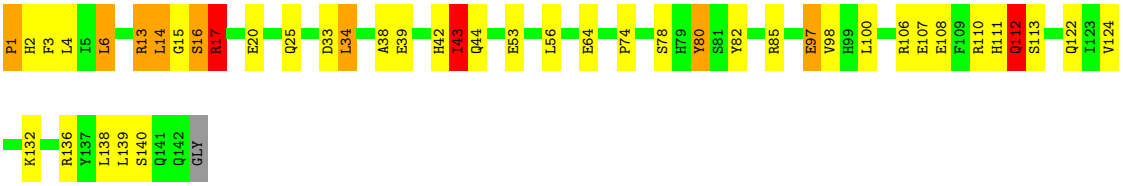
• Molecule 1: DEHYDROQUINASE

Chain O:



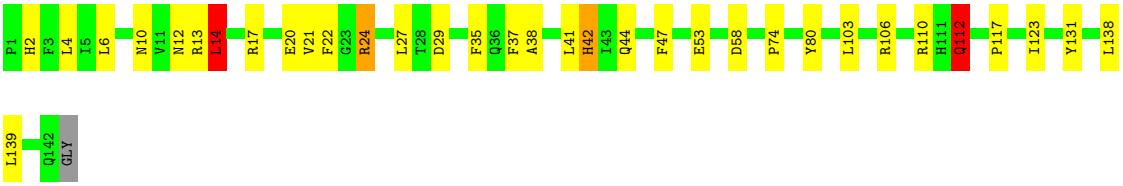
• Molecule 1: DEHYDROQUINASE

Chain P:



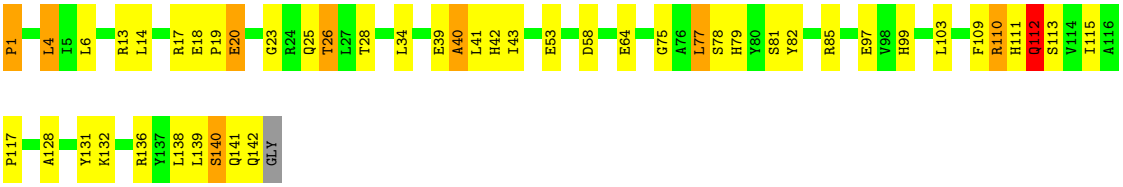
• Molecule 1: DEHYDROQUINASE

Chain Q:



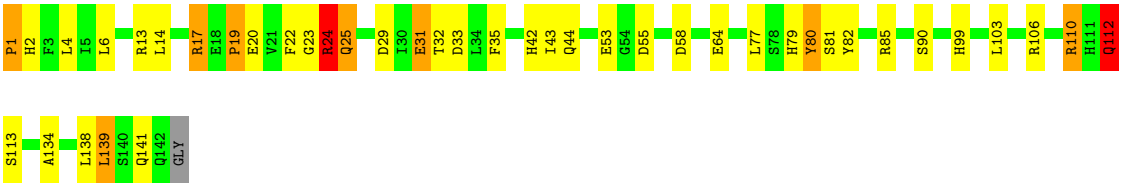
• Molecule 1: DEHYDROQUINASE

Chain R:



• Molecule 1: DEHYDROQUINASE

Chain S:

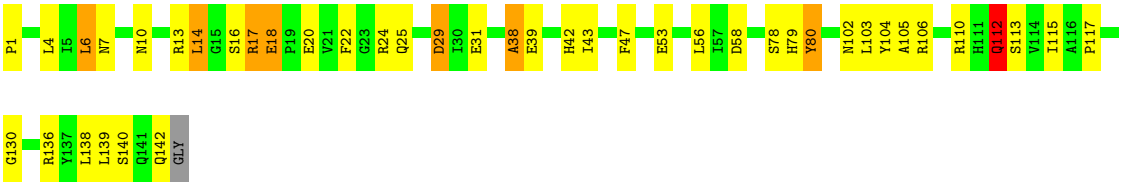


• Molecule 1: DEHYDROQUINASE

Chain T:

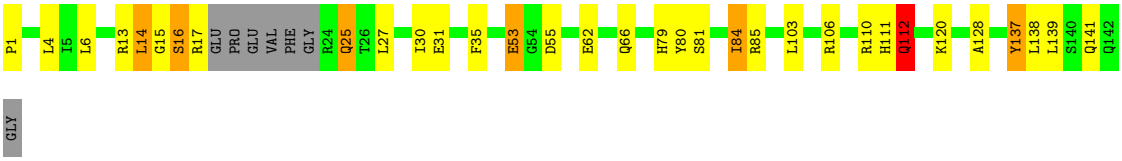
• Molecule 1: DEHYDROQUINASE

Chain U:



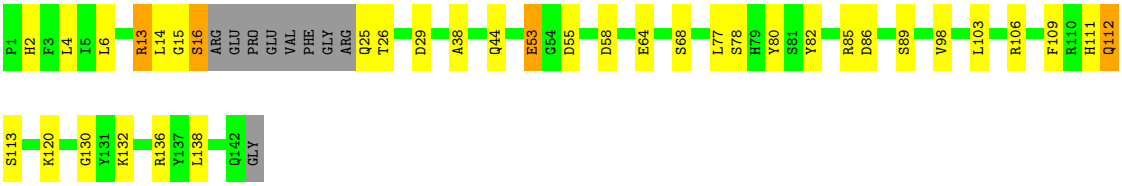
• Molecule 1: DEHYDROQUINASE

Chain V:



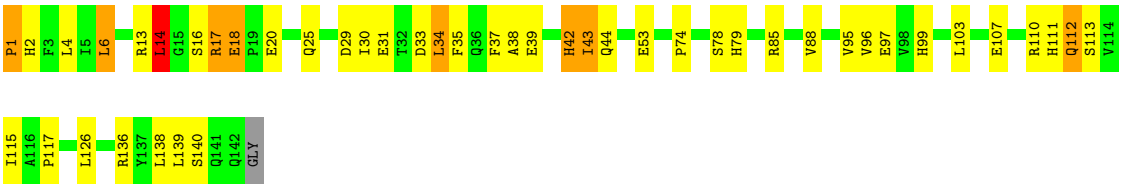
• Molecule 1: DEHYDROQUINASE

Chain X:



• Molecule 1: DEHYDROQUINASE

Chain Y:



4 Data and refinement statistics (i)

Xtriage (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	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(^{o})	Ideal(^{o})
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 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	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
2	R	18	0	24	6	0
2	S	18	0	24	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 11.

The worst 5 of 589 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: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	Interatomic distance (Å)	Clash overlap (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 (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	139/143 (97%)	131 (94%)	8 (6%)	0	100 100
1	B	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	22 18
1	C	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	D	140/143 (98%)	132 (94%)	7 (5%)	1 (1%)	22 18
1	E	142/143 (99%)	130 (92%)	10 (7%)	2 (1%)	11 6
1	F	142/143 (99%)	133 (94%)	7 (5%)	2 (1%)	11 6
1	G	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	11 6
1	H	140/143 (98%)	132 (94%)	8 (6%)	0	100 100
1	I	139/143 (97%)	130 (94%)	5 (4%)	4 (3%)	4 1
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%)	2 0
1	M	140/143 (98%)	133 (95%)	5 (4%)	2 (1%)	11 6
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%)	11 6
1	Q	139/143 (97%)	132 (95%)	7 (5%)	0	100 100
1	R	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	22 18
1	S	139/143 (97%)	132 (95%)	7 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	T	140/143 (98%)	133 (95%)	6 (4%)	1 (1%)	22 18
1	U	139/143 (97%)	131 (94%)	6 (4%)	2 (1%)	11 6
1	V	131/143 (92%)	125 (95%)	5 (4%)	1 (1%)	19 15
1	X	129/143 (90%)	122 (95%)	7 (5%)	0	100 100
1	Y	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	22 18
All	All	3314/3432 (97%)	3130 (94%)	156 (5%)	28 (1%)	19 15

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 (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	115/120 (96%)	105 (91%)	10 (9%)	10 7
1	B	115/120 (96%)	106 (92%)	9 (8%)	12 9
1	C	115/120 (96%)	108 (94%)	7 (6%)	18 16
1	D	115/120 (96%)	102 (89%)	13 (11%)	6 3
1	E	119/120 (99%)	110 (92%)	9 (8%)	13 10
1	F	119/120 (99%)	112 (94%)	7 (6%)	19 17
1	G	117/120 (98%)	108 (92%)	9 (8%)	13 9
1	H	115/120 (96%)	102 (89%)	13 (11%)	6 3
1	I	114/120 (95%)	105 (92%)	9 (8%)	12 9
1	J	115/120 (96%)	107 (93%)	8 (7%)	15 12
1	K	110/120 (92%)	101 (92%)	9 (8%)	11 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	113/120 (94%)	104 (92%)	9 (8%)	12 8
1	M	116/120 (97%)	107 (92%)	9 (8%)	12 9
1	N	109/120 (91%)	102 (94%)	7 (6%)	17 14
1	O	115/120 (96%)	108 (94%)	7 (6%)	18 16
1	P	116/120 (97%)	105 (90%)	11 (10%)	8 5
1	Q	118/120 (98%)	110 (93%)	8 (7%)	16 13
1	R	115/120 (96%)	105 (91%)	10 (9%)	10 7
1	S	118/120 (98%)	105 (89%)	13 (11%)	6 3
1	T	118/120 (98%)	108 (92%)	10 (8%)	10 7
1	U	115/120 (96%)	108 (94%)	7 (6%)	18 16
1	V	112/120 (93%)	105 (94%)	7 (6%)	18 15
1	X	110/120 (92%)	103 (94%)	7 (6%)	17 14
1	Y	115/120 (96%)	100 (87%)	15 (13%)	4 2
All	All	2759/2880 (96%)	2536 (92%)	223 (8%)	12 8

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

Mol	Chain	Res	Type
1	M	17	ARG
1	Y	138	LEU
1	P	112	GLN
1	Y	74	PRO
1	V	112	GLN

Sometimes 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	U	66	GLN
1	M	66	GLN
1	V	66	GLN
1	S	25	GLN

5.3.3 RNA

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)

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	D	151	-	5,5,5	0.90	0	5,5,5	0.74	0
2	GOL	V	152	-	5,5,5	0.74	0	5,5,5	1.33	0
2	GOL	E	151	-	5,5,5	0.63	0	5,5,5	0.84	0
2	GOL	I	152	-	5,5,5	0.57	0	5,5,5	1.04	0
2	GOL	L	152	-	5,5,5	0.56	0	5,5,5	1.16	0
2	GOL	K	151	-	5,5,5	0.70	0	5,5,5	0.62	0
2	GOL	G	151	-	5,5,5	0.65	0	5,5,5	1.47	1 (20%)
2	GOL	U	150	-	5,5,5	0.99	0	5,5,5	1.53	1 (20%)
2	GOL	P	152	-	5,5,5	0.71	0	5,5,5	0.72	0
2	GOL	I	151	-	5,5,5	0.63	0	5,5,5	0.93	0
2	GOL	L	150	-	5,5,5	0.98	1 (20%)	5,5,5	2.33	2 (40%)
2	GOL	D	152	-	5,5,5	0.52	0	5,5,5	2.02	4 (80%)
2	GOL	U	151	-	5,5,5	0.43	0	5,5,5	0.80	0
2	GOL	G	150	-	5,5,5	0.59	0	5,5,5	1.19	1 (20%)
2	GOL	V	150	-	5,5,5	0.61	0	5,5,5	1.14	1 (20%)
2	GOL	L	151	-	5,5,5	0.58	0	5,5,5	0.86	0
2	GOL	Y	152	-	5,5,5	1.00	0	5,5,5	0.76	0
2	GOL	S	152	-	5,5,5	0.62	0	5,5,5	1.00	0
2	GOL	P	151	-	5,5,5	0.79	0	5,5,5	0.83	0
2	GOL	Y	150	-	5,5,5	0.71	0	5,5,5	1.68	2 (40%)
2	GOL	J	150	-	5,5,5	0.95	0	5,5,5	2.40	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	A	150	-	5,5,5	0.97	0	5,5,5	0.52	0
2	GOL	O	151	-	5,5,5	0.85	0	5,5,5	1.13	1 (20%)
2	GOL	J	151	-	5,5,5	0.71	0	5,5,5	1.32	1 (20%)
2	GOL	Q	150	-	5,5,5	1.15	0	5,5,5	1.51	1 (20%)
2	GOL	K	152	-	5,5,5	0.82	0	5,5,5	1.04	0
2	GOL	K	150	-	5,5,5	1.11	1 (20%)	5,5,5	1.25	0
2	GOL	C	152	-	5,5,5	0.83	0	5,5,5	0.72	0
2	GOL	S	151	-	5,5,5	0.80	0	5,5,5	1.80	2 (40%)
2	GOL	T	151	-	5,5,5	0.67	0	5,5,5	0.55	0
2	GOL	X	152	-	5,5,5	0.85	0	5,5,5	0.46	0
2	GOL	E	152	-	4,4,5	0.95	0	4,4,5	0.77	0
2	GOL	T	152	-	5,5,5	0.72	0	5,5,5	0.75	0
2	GOL	H	152	-	5,5,5	0.83	0	5,5,5	1.20	0
2	GOL	X	150	-	5,5,5	1.40	1 (20%)	5,5,5	1.08	0
2	GOL	D	150	-	5,5,5	1.05	0	5,5,5	2.34	2 (40%)
2	GOL	O	152	-	5,5,5	0.79	0	5,5,5	0.57	0
2	GOL	C	151	-	5,5,5	0.82	0	5,5,5	1.04	0
2	GOL	H	150	-	5,5,5	0.96	0	5,5,5	1.50	1 (20%)
2	GOL	R	150	-	5,5,5	1.89	2 (40%)	5,5,5	2.39	3 (60%)
2	GOL	S	150	-	5,5,5	1.86	1 (20%)	5,5,5	1.48	1 (20%)
2	GOL	T	150	-	5,5,5	1.07	0	5,5,5	1.70	1 (20%)
2	GOL	E	150	-	5,5,5	1.11	1 (20%)	5,5,5	0.93	0
2	GOL	A	152	-	5,5,5	0.77	0	5,5,5	1.03	0
2	GOL	P	150	-	5,5,5	1.18	1 (20%)	5,5,5	1.18	0
2	GOL	R	151	-	5,5,5	0.47	0	5,5,5	1.53	2 (40%)
2	GOL	C	150	-	5,5,5	1.12	0	5,5,5	1.29	1 (20%)
2	GOL	I	150	-	5,5,5	0.79	0	5,5,5	1.75	3 (60%)
2	GOL	H	151	-	5,5,5	0.77	0	5,5,5	0.80	0
2	GOL	N	151	-	5,5,5	0.75	0	5,5,5	1.55	1 (20%)
2	GOL	N	152	-	5,5,5	0.69	0	5,5,5	0.91	0
2	GOL	J	152	-	5,5,5	0.83	0	5,5,5	1.14	1 (20%)
2	GOL	Q	152	-	5,5,5	0.96	0	5,5,5	0.77	0
2	GOL	M	151	-	5,5,5	0.63	0	5,5,5	0.94	0
2	GOL	F	152	-	4,4,5	1.13	0	4,4,5	0.75	0
2	GOL	N	150	-	5,5,5	1.20	0	5,5,5	1.58	1 (20%)
2	GOL	A	151	-	5,5,5	0.70	0	5,5,5	2.11	2 (40%)
2	GOL	B	151	-	5,5,5	0.90	0	5,5,5	1.26	1 (20%)
2	GOL	B	152	-	5,5,5	0.68	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	F	150	-	5,5,5	1.18	0	5,5,5	1.88	3 (60%)
2	GOL	M	152	-	5,5,5	0.54	0	5,5,5	0.99	0
2	GOL	O	150	-	5,5,5	1.30	1 (20%)	5,5,5	1.78	1 (20%)
2	GOL	X	151	-	5,5,5	0.79	0	5,5,5	1.72	1 (20%)
2	GOL	F	151	-	5,5,5	0.60	0	5,5,5	0.82	0
2	GOL	Q	151	-	5,5,5	0.78	0	5,5,5	0.52	0
2	GOL	B	150	-	5,5,5	0.84	0	5,5,5	1.21	0
2	GOL	R	152	-	5,5,5	0.68	0	5,5,5	0.80	0
2	GOL	Y	151	-	5,5,5	0.56	0	5,5,5	0.94	0
2	GOL	M	150	-	5,5,5	1.11	0	5,5,5	1.25	0
2	GOL	U	152	-	5,5,5	0.79	0	5,5,5	0.70	0
2	GOL	G	152	-	5,5,5	0.72	0	5,5,5	1.94	2 (40%)
2	GOL	V	151	-	5,5,5	0.73	0	5,5,5	2.00	1 (20%)

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	D	151	-	-	4/4/4/4	-
2	GOL	V	152	-	-	4/4/4/4	-
2	GOL	E	151	-	-	4/4/4/4	-
2	GOL	I	152	-	-	2/4/4/4	-
2	GOL	L	152	-	-	2/4/4/4	-
2	GOL	K	151	-	-	2/4/4/4	-
2	GOL	G	151	-	-	1/4/4/4	-
2	GOL	U	150	-	-	4/4/4/4	-
2	GOL	P	152	-	-	4/4/4/4	-
2	GOL	I	151	-	-	3/4/4/4	-
2	GOL	L	150	-	-	3/4/4/4	-
2	GOL	D	152	-	-	3/4/4/4	-
2	GOL	U	151	-	-	4/4/4/4	-
2	GOL	G	150	-	-	0/4/4/4	-
2	GOL	V	150	-	-	3/4/4/4	-
2	GOL	L	151	-	-	2/4/4/4	-
2	GOL	Y	152	-	-	1/4/4/4	-
2	GOL	S	152	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	P	151	-	-	4/4/4/4	-
2	GOL	Y	150	-	-	1/4/4/4	-
2	GOL	J	150	-	-	2/4/4/4	-
2	GOL	A	150	-	-	2/4/4/4	-
2	GOL	O	151	-	-	2/4/4/4	-
2	GOL	J	151	-	-	2/4/4/4	-
2	GOL	Q	150	-	-	2/4/4/4	-
2	GOL	K	152	-	-	1/4/4/4	-
2	GOL	K	150	-	-	1/4/4/4	-
2	GOL	C	152	-	-	0/4/4/4	-
2	GOL	S	151	-	-	2/4/4/4	-
2	GOL	T	151	-	-	2/4/4/4	-
2	GOL	X	152	-	-	2/4/4/4	-
2	GOL	E	152	-	-	0/2/2/4	-
2	GOL	T	152	-	-	2/4/4/4	-
2	GOL	H	152	-	-	2/4/4/4	-
2	GOL	X	150	-	-	4/4/4/4	-
2	GOL	D	150	-	-	2/4/4/4	-
2	GOL	O	152	-	-	2/4/4/4	-
2	GOL	C	151	-	-	2/4/4/4	-
2	GOL	H	150	-	-	2/4/4/4	-
2	GOL	R	150	-	-	2/4/4/4	-
2	GOL	S	150	-	-	4/4/4/4	-
2	GOL	T	150	-	-	2/4/4/4	-
2	GOL	E	150	-	-	1/4/4/4	-
2	GOL	A	152	-	-	4/4/4/4	-
2	GOL	P	150	-	-	3/4/4/4	-
2	GOL	R	151	-	-	1/4/4/4	-
2	GOL	C	150	-	-	2/4/4/4	-
2	GOL	I	150	-	-	3/4/4/4	-
2	GOL	H	151	-	-	2/4/4/4	-
2	GOL	N	151	-	-	4/4/4/4	-
2	GOL	N	152	-	-	4/4/4/4	-
2	GOL	J	152	-	-	2/4/4/4	-
2	GOL	Q	152	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	M	151	-	-	3/4/4/4	-
2	GOL	F	152	-	-	2/2/2/4	-
2	GOL	N	150	-	-	2/4/4/4	-
2	GOL	A	151	-	-	3/4/4/4	-
2	GOL	B	151	-	-	2/4/4/4	-
2	GOL	B	152	-	-	4/4/4/4	-
2	GOL	F	150	-	-	3/4/4/4	-
2	GOL	M	152	-	-	3/4/4/4	-
2	GOL	O	150	-	-	4/4/4/4	-
2	GOL	X	151	-	-	1/4/4/4	-
2	GOL	F	151	-	-	3/4/4/4	-
2	GOL	Q	151	-	-	4/4/4/4	-
2	GOL	B	150	-	-	2/4/4/4	-
2	GOL	R	152	-	-	1/4/4/4	-
2	GOL	Y	151	-	-	2/4/4/4	-
2	GOL	M	150	-	-	4/4/4/4	-
2	GOL	U	152	-	-	2/4/4/4	-
2	GOL	G	152	-	-	3/4/4/4	-
2	GOL	V	151	-	-	3/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	150	GOL	O1-C1	3.67	1.57	1.42
2	R	150	GOL	C1-C2	2.77	1.62	1.51
2	X	150	GOL	O1-C1	2.71	1.53	1.42
2	E	150	GOL	C1-C2	2.16	1.60	1.51
2	O	150	GOL	C1-C2	2.15	1.60	1.51

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	150	GOL	C3-C2-C1	4.32	127.66	111.80
2	V	151	GOL	O2-C2-C1	3.99	125.71	109.18
2	L	150	GOL	C3-C2-C1	3.85	125.92	111.80
2	D	150	GOL	O1-C1-C2	-3.62	94.07	110.38
2	A	151	GOL	O2-C2-C1	3.50	123.68	109.18

There are no chirality outliers.

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	150	GOL	C1-C2-C3-O3
2	A	151	GOL	O1-C1-C2-C3
2	A	152	GOL	C1-C2-C3-O3
2	B	150	GOL	O1-C1-C2-C3
2	B	152	GOL	C1-C2-C3-O3

There are no ring outliers.

53 monomers are involved in 133 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	151	GOL	4	0
2	V	152	GOL	2	0
2	E	151	GOL	1	0
2	I	152	GOL	2	0
2	L	152	GOL	3	0
2	K	151	GOL	2	0
2	G	151	GOL	5	0
2	P	152	GOL	1	0
2	I	151	GOL	2	0
2	L	150	GOL	2	0
2	D	152	GOL	1	0
2	U	151	GOL	8	0
2	L	151	GOL	4	0
2	Y	152	GOL	1	0
2	S	152	GOL	4	0
2	P	151	GOL	5	0
2	Y	150	GOL	1	0
2	A	150	GOL	1	0
2	O	151	GOL	4	0
2	J	151	GOL	2	0
2	K	152	GOL	4	0
2	C	152	GOL	3	0
2	S	151	GOL	4	0
2	T	151	GOL	1	0
2	E	152	GOL	1	0
2	T	152	GOL	3	0
2	H	152	GOL	2	0
2	X	150	GOL	1	0
2	O	152	GOL	4	0
2	C	151	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	150	GOL	1	0
2	S	150	GOL	3	0
2	E	150	GOL	1	0
2	A	152	GOL	2	0
2	R	151	GOL	5	0
2	H	151	GOL	2	0
2	N	151	GOL	1	0
2	N	152	GOL	2	0
2	Q	152	GOL	3	0
2	M	151	GOL	1	0
2	F	152	GOL	1	0
2	A	151	GOL	2	0
2	B	151	GOL	3	0
2	B	152	GOL	2	0
2	M	152	GOL	2	0
2	X	151	GOL	2	0
2	F	151	GOL	2	0
2	Q	151	GOL	8	0
2	R	152	GOL	1	0
2	Y	151	GOL	5	0
2	U	152	GOL	2	0
2	G	152	GOL	1	0
2	V	151	GOL	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	O	1
1	C	1
1	D	1
1	P	1
1	L	1
1	Q	1
1	I	1

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Mol	Chain	Number of breaks
1	U	1
1	S	1
1	A	1
1	R	1
1	Y	1
1	F	1
1	T	1
1	N	1
1	G	1
1	X	1
1	V	1
1	J	1
1	K	1
1	M	1
1	H	1
1	E	1

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	O	141:GLN	C	142:GLN	N	5.77
1	C	141:GLN	C	142:GLN	N	5.67
1	D	141:GLN	C	142:GLN	N	5.59
1	P	141:GLN	C	142:GLN	N	5.45
1	L	141:GLN	C	142:GLN	N	5.26

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.