



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 PM GMT

PDB ID : 4LRX  
Title : Crystal Structure of the E.coli DhaR(N)-DhaK complex  
Authors : Shi, R.; McDonald, L.; Cygler, M.; Ekiel, I.  
Deposited on : 2013-07-21  
Resolution : 3.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

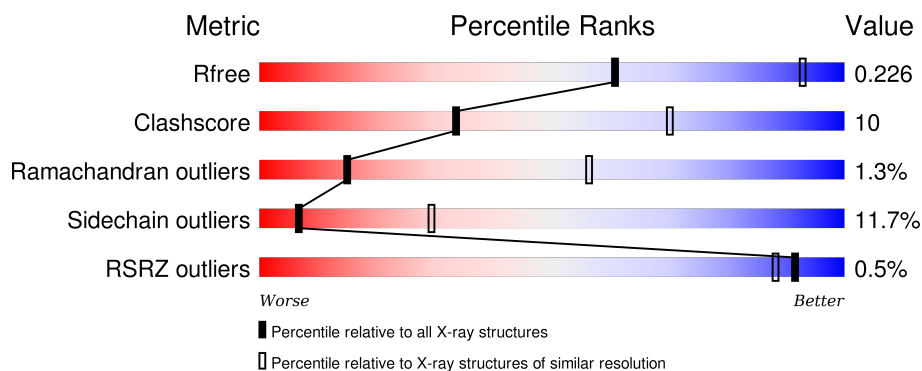
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	356	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>76% 22% .</div>
1	B	356	<div> <div style="width: 77%; background-color: green;"></div> <div style="width: 22%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>77% 22% .</div>
2	C	318	<div> <div style="width: 59%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 7%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>% 59% 30% . 7%</div>
2	D	318	<div> <div style="width: 62%; background-color: green;"></div> <div style="width: 24%; background-color: yellow;"></div> <div style="width: 5%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>62% 24% 5% . 7%</div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	401	-	-	X	-
3	GOL	B	401	-	-	X	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9912 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 PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2681	1679	460	529	13			
1	B	356	Total	C	N	O	S	0	0	0
			2681	1679	460	529	13			

- Molecule 2 is a protein called PTS-dependent dihydroxyacetone kinase operon regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	295	Total	C	N	O	S	0	0	0
			2269	1438	393	426	12			
2	D	295	Total	C	N	O	S	0	0	0
			2269	1438	393	426	12			

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

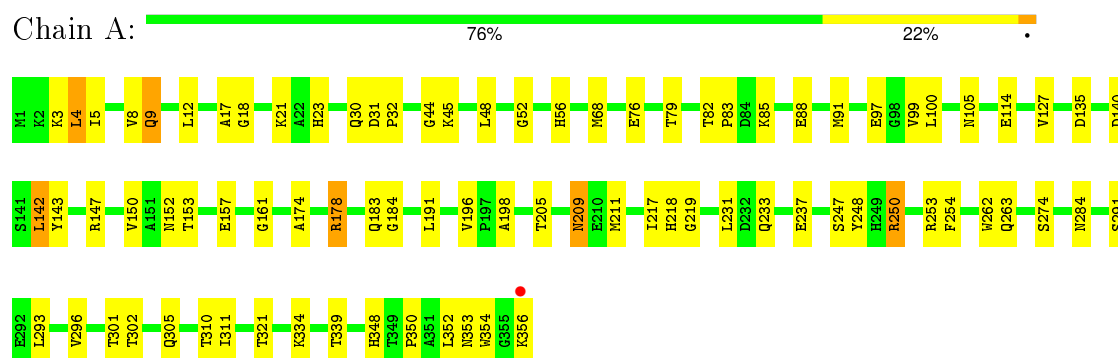


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

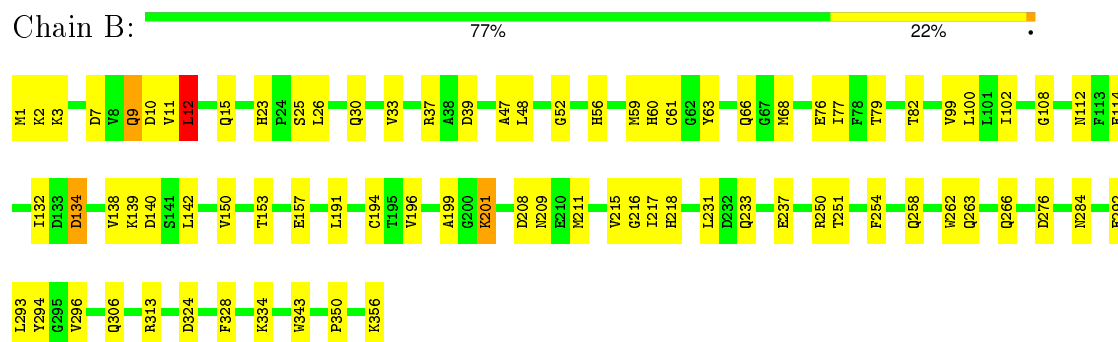
### 3 Residue-property plots

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.

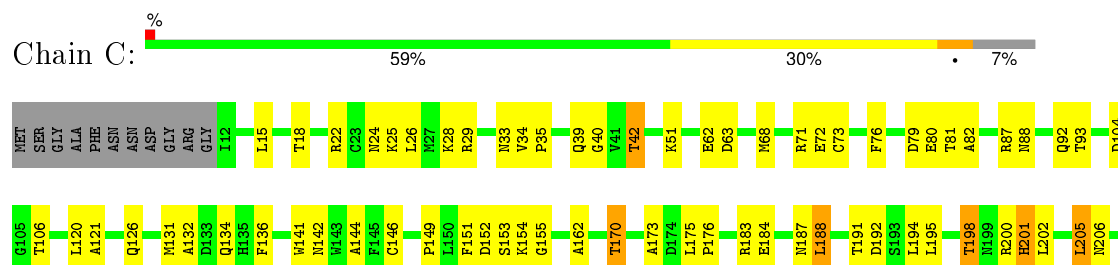
- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK

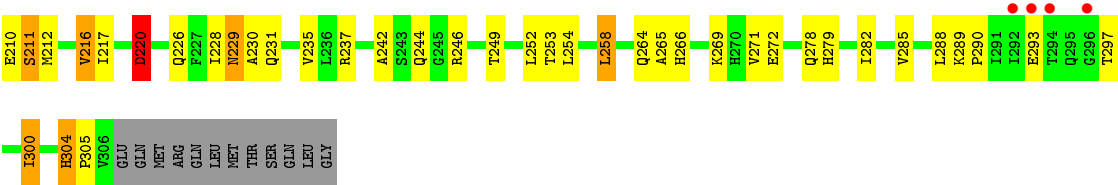


- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK

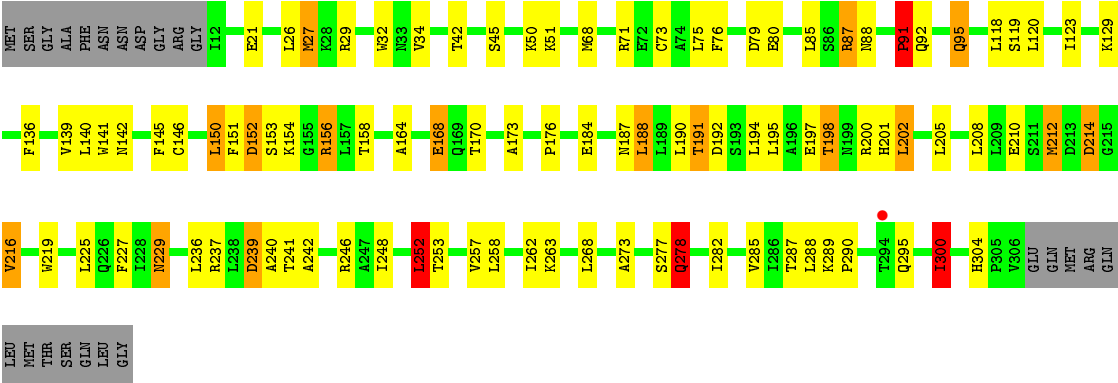


- Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein





● Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	232.13 Å   232.13 Å   79.89 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	50.00 – 3.25 46.95 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-3.25) 99.6 (46.95-3.25)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.25 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.191 , 0.228 0.188 , 0.226	Depositor DCC
$R_{free}$ test set	1957 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 15.4	EDS
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39037 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9912	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	0/2730	0.74	0/3710
1	B	0.63	0/2730	0.74	2/3710 (0.1%)
2	C	0.77	2/2311 (0.1%)	0.83	1/3147 (0.0%)
2	D	0.77	1/2311 (0.0%)	0.86	3/3147 (0.1%)
All	All	0.70	3/10082 (0.0%)	0.79	6/13714 (0.0%)

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
2	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	304	HIS	CB-CG	-6.30	1.38	1.50
2	C	62	GLU	CG-CD	5.76	1.60	1.51
2	D	273	ALA	C-O	-5.63	1.12	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	ILE	CB-CA-C	-5.98	99.64	111.60
1	B	12	LEU	CA-CB-CG	-5.82	101.92	115.30
2	D	152	ASP	N-CA-CB	-5.75	100.26	110.60
2	C	271	VAL	CA-CB-CG2	-5.50	102.66	110.90
1	B	61	CYS	CA-CB-SG	-5.49	104.12	114.00
2	D	252	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	151	PHE	Peptide

## 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	2681	0	2637	46	0
1	B	2681	0	2637	48	0
2	C	2269	0	2282	68	0
2	D	2269	0	2282	72	0
3	A	6	0	8	6	0
3	B	6	0	8	5	0
All	All	9912	0	9854	202	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 10.

All (202) 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:B:218:HIS:NE2	3:B:401:GOL:H2	1.50	1.25
1:A:218:HIS:NE2	3:A:401:GOL:H2	1.66	1.10
2:D:68:MET:HE2	2:D:71:ARG:HH11	1.01	1.09
2:C:211:SER:HB3	2:D:300:ILE:HD11	1.08	1.07
1:B:218:HIS:NE2	3:B:401:GOL:C2	2.20	1.04
1:A:88:GLU:OE2	2:C:42:THR:HG21	1.58	1.04
2:D:216:VAL:H	2:D:229:ASN:ND2	1.55	1.03
1:A:218:HIS:CE1	3:A:401:GOL:H2	1.94	1.00
2:C:211:SER:CB	2:D:300:ILE:HD11	1.92	0.99
1:B:218:HIS:CE1	3:B:401:GOL:H2	2.00	0.96
2:C:217:ILE:HG12	2:C:228:ILE:HG13	1.49	0.94
1:A:218:HIS:NE2	3:A:401:GOL:C2	2.31	0.93
2:D:68:MET:HE2	2:D:71:ARG:NH1	1.83	0.93
2:D:216:VAL:N	2:D:229:ASN:HD21	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:O	1:A:157:GLU:HG3	1.73	0.89
2:C:211:SER:HB3	2:D:300:ILE:CD1	2.00	0.86
2:C:131:MET:O	2:C:134:GLN:HG3	1.76	0.84
2:D:150:LEU:O	2:D:158:THR:HG22	1.79	0.83
2:C:220:ASP:OD1	2:C:226:GLN:NE2	2.15	0.79
2:D:216:VAL:H	2:D:229:ASN:HD21	0.84	0.78
1:A:284:ASN:HB2	1:A:293:LEU:HD11	1.64	0.77
2:D:68:MET:CE	2:D:71:ARG:HH11	1.92	0.76
2:D:92:GLN:HA	2:D:95:GLN:HG3	1.67	0.76
2:C:235:VAL:O	2:C:282:ILE:HD12	1.87	0.74
1:B:9:GLN:HE21	1:B:9:GLN:H	1.36	0.71
2:C:29:ARG:HG2	2:C:136:PHE:O	1.91	0.71
2:C:29:ARG:NH1	2:C:141:TRP:HZ2	1.88	0.70
2:D:214:ASP:OD1	2:D:304:HIS:ND1	2.22	0.70
1:A:233:GLN:O	1:A:237:GLU:HG2	1.94	0.67
2:D:79:ASP:HB3	2:D:85:LEU:HD11	1.76	0.66
1:B:218:HIS:NE2	3:B:401:GOL:O2	2.28	0.66
1:B:12:LEU:HD11	1:B:77:ILE:HG13	1.79	0.65
1:B:284:ASN:HB2	1:B:293:LEU:HD11	1.80	0.64
2:D:152:ASP:HB2	2:D:156:ARG:O	1.98	0.63
2:C:217:ILE:CG1	2:C:228:ILE:HG13	2.28	0.62
2:D:210:GLU:OE2	2:D:229:ASN:HB2	2.00	0.62
1:A:31:ASP:HB3	2:C:39:GLN:OE1	1.99	0.62
2:D:32:TRP:HB2	2:D:139:VAL:HG21	1.80	0.62
2:D:239:ASP:OD2	2:D:242:ALA:HB3	1.99	0.62
2:C:71:ARG:HG2	2:C:72:GLU:N	2.14	0.61
1:B:48:LEU:HD11	1:B:102:ILE:HD11	1.82	0.61
1:A:23:HIS:CE1	1:A:350:PRO:HB3	2.34	0.61
1:A:219:GLY:O	2:C:25:LYS:HE2	2.00	0.61
1:A:44:GLY:O	1:A:97:GLU:HG3	2.01	0.61
2:D:201:HIS:HD2	2:D:205:LEU:HD13	1.66	0.61
2:C:194:LEU:O	2:C:198:THR:HG23	2.01	0.60
2:D:194:LEU:O	2:D:198:THR:HG23	2.00	0.60
2:C:173:ALA:HB3	2:D:173:ALA:HB3	1.84	0.60
1:B:231:LEU:HD11	1:B:296:VAL:CG2	2.32	0.60
1:B:11:VAL:O	1:B:15:GLN:HG3	2.01	0.60
2:C:173:ALA:O	2:C:176:PRO:HD2	2.03	0.59
2:C:29:ARG:NH1	2:C:141:TRP:CZ2	2.70	0.59
1:B:231:LEU:CD1	1:B:296:VAL:HG22	2.33	0.59
1:A:218:HIS:NE2	3:A:401:GOL:O2	2.36	0.58
2:C:68:MET:HE3	2:D:173:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:HA	1:A:321:THR:O	2.04	0.58
2:D:227:PHE:HE2	2:D:229:ASN:HB3	1.69	0.57
2:C:237:ARG:HE	2:C:282:ILE:HD11	1.70	0.57
2:D:29:ARG:NH1	2:D:141:TRP:HZ2	2.03	0.56
1:B:37:ARG:NH2	1:B:66:GLN:HA	2.20	0.56
1:A:32:PRO:HB2	1:A:85:LYS:HG2	1.88	0.55
2:C:200:ARG:HH12	2:D:295:GLN:NE2	2.04	0.55
2:D:32:TRP:CB	2:D:139:VAL:HG21	2.37	0.54
1:B:231:LEU:HD11	1:B:296:VAL:HG22	1.88	0.54
1:A:301:THR:HG22	1:A:311:ILE:HD12	1.90	0.54
2:D:129:LYS:HG3	2:D:146:CYS:SG	2.48	0.54
2:D:201:HIS:CD2	2:D:205:LEU:HD13	2.43	0.54
1:B:313:ARG:HG3	1:B:343:TRP:CD1	2.43	0.54
2:C:81:THR:O	2:C:82:ALA:HB3	2.08	0.54
1:A:254:PHE:CZ	1:A:263:GLN:HG2	2.43	0.54
1:A:174:ALA:O	1:A:178:ARG:HB2	2.08	0.54
2:C:68:MET:CE	2:D:173:ALA:HA	2.38	0.53
2:C:68:MET:HB2	2:D:176:PRO:HG3	1.89	0.53
1:B:231:LEU:CD1	1:B:296:VAL:CG2	2.86	0.53
2:D:76:PHE:CD1	2:D:87:ARG:HB3	2.43	0.53
1:A:191:LEU:HD23	1:A:211:MET:HB3	1.90	0.53
2:D:229:ASN:HD22	2:D:229:ASN:H	1.57	0.53
2:C:76:PHE:CE1	2:C:87:ARG:HG2	2.44	0.52
1:A:4:LEU:HD21	1:B:328:PHE:HE2	1.74	0.52
2:D:227:PHE:CE2	2:D:229:ASN:HB3	2.43	0.52
2:C:212:MET:CE	2:D:212:MET:CE	2.87	0.52
1:B:48:LEU:CD1	1:B:100:LEU:HD23	2.39	0.52
1:A:4:LEU:CD2	1:B:328:PHE:HE2	2.22	0.52
1:B:30:GLN:HA	1:B:30:GLN:HE21	1.74	0.52
2:C:216:VAL:H	2:C:229:ASN:ND2	2.08	0.52
2:C:132:ALA:HA	2:C:141:TRP:O	2.10	0.52
1:A:218:HIS:CE1	3:A:401:GOL:C2	2.80	0.51
2:C:212:MET:HE2	2:D:212:MET:HE2	1.91	0.51
2:D:140:LEU:HD22	2:D:145:PHE:HE2	1.76	0.51
1:A:142:LEU:HD22	2:C:22:ARG:HG2	1.93	0.50
1:A:114:GLU:HG2	1:A:262:TRP:CH2	2.45	0.50
1:B:153:THR:O	1:B:157:GLU:HG3	2.11	0.50
2:D:26:LEU:O	2:D:27:MET:HB2	2.09	0.50
1:A:17:ALA:O	1:A:21:LYS:HG3	2.12	0.50
2:C:278:GLN:O	2:C:279:HIS:HB2	2.10	0.50
1:B:9:GLN:NE2	1:B:9:GLN:H	2.08	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:HIS:CE1	1:B:350:PRO:HB3	2.47	0.49
1:B:56:HIS:CE1	1:B:217:ILE:HD12	2.47	0.49
2:C:212:MET:HG3	2:D:212:MET:HE3	1.94	0.49
1:A:198:ALA:O	2:C:28:LYS:HG3	2.12	0.49
2:C:79:ASP:OD1	2:C:79:ASP:C	2.50	0.48
2:C:254:LEU:HD22	2:C:258:LEU:HD13	1.95	0.48
2:D:236:LEU:HD13	2:D:252:LEU:HD11	1.96	0.48
2:D:188:LEU:O	2:D:192:ASP:HB2	2.13	0.48
2:C:212:MET:CE	2:D:212:MET:HE3	2.44	0.48
2:D:73:CYS:HB2	2:D:164:ALA:O	2.14	0.48
2:C:87:ARG:HD3	2:C:104:ASP:OD2	2.14	0.48
2:C:146:CYS:O	2:C:162:ALA:HA	2.14	0.48
2:C:187:ASN:HB3	2:D:188:LEU:HD21	1.96	0.47
2:C:206:ASN:ND2	2:C:210:GLU:HG2	2.29	0.47
2:D:29:ARG:HG2	2:D:136:PHE:O	2.14	0.47
2:C:188:LEU:O	2:C:192:ASP:HB2	2.13	0.47
1:B:134:ASP:OD1	1:B:134:ASP:N	2.44	0.47
1:A:9:GLN:H	1:A:9:GLN:NE2	2.13	0.47
1:A:209:ASN:HD21	1:B:1:MET:CG	2.27	0.47
1:B:52:GLY:HA3	3:B:401:GOL:O1	2.15	0.46
1:A:48:LEU:HD12	1:A:100:LEU:HB3	1.96	0.46
1:A:152:ASN:ND2	1:A:184:GLY:HA3	2.31	0.46
2:C:183:ARG:O	2:C:187:ASN:HB2	2.16	0.46
1:A:231:LEU:HD11	1:A:296:VAL:HG22	1.98	0.46
2:C:188:LEU:HD13	2:D:188:LEU:HD13	1.98	0.46
2:D:187:ASN:O	2:D:191:THR:HG23	2.16	0.46
2:D:91:PRO:O	2:D:95:GLN:HG2	2.16	0.46
1:A:105:ASN:ND2	1:A:147:ARG:O	2.47	0.46
2:C:175:LEU:HD12	2:C:175:LEU:HA	1.72	0.46
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.31	0.45
1:B:276:ASP:OD1	1:B:334:LYS:HD2	2.15	0.45
1:A:4:LEU:HB2	1:B:292:GLU:OE1	2.15	0.45
1:B:215:VAL:HG22	1:B:216:GLY:N	2.31	0.45
2:D:119:SER:O	2:D:123:ILE:HD12	2.16	0.45
2:D:188:LEU:HA	2:D:188:LEU:HD12	1.87	0.45
2:C:173:ALA:C	2:C:176:PRO:HD2	2.37	0.45
2:C:212:MET:HE3	2:D:212:MET:HG3	1.97	0.45
2:D:29:ARG:HH12	2:D:141:TRP:HZ2	1.64	0.45
1:A:183:GLN:HB3	1:A:334:LYS:HB3	1.97	0.45
1:A:83:PRO:HG3	2:C:81:THR:HG21	1.99	0.45
1:A:18:GLY:HA3	1:B:294:TYR:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:PHE:CE1	2:D:87:ARG:HB3	2.52	0.45
1:B:76:GLU:HB2	1:B:79:THR:OG1	2.17	0.44
1:B:194:CYS:HA	1:B:324:ASP:OD1	2.17	0.44
1:A:76:GLU:HB2	1:A:79:THR:HB	1.99	0.44
2:D:168:GLU:CD	2:D:168:GLU:H	2.20	0.44
1:A:352:LEU:HD22	1:A:354:TRP:CZ3	2.52	0.44
1:B:108:GLY:O	1:B:112:ASN:ND2	2.50	0.44
1:B:37:ARG:HB3	1:B:39:ASP:OD1	2.18	0.44
2:D:216:VAL:HG13	2:D:229:ASN:ND2	2.33	0.43
1:B:208:ASP:O	1:B:209:ASN:C	2.55	0.43
1:A:248:TYR:CE2	1:A:250:ARG:HD2	2.52	0.43
2:C:304:HIS:HA	2:C:305:PRO:HD3	1.91	0.43
2:C:212:MET:HE2	2:D:212:MET:CE	2.48	0.43
2:C:212:MET:HE3	2:D:212:MET:CE	2.48	0.43
1:A:68:MET:HA	1:A:161:GLY:HA3	2.01	0.43
2:C:184:GLU:O	2:C:188:LEU:HB2	2.19	0.43
2:C:289:LYS:HA	2:C:290:PRO:HD3	1.86	0.43
2:D:288:LEU:HD12	2:D:300:ILE:O	2.19	0.43
2:D:152:ASP:HB3	2:D:156:ARG:N	2.34	0.43
2:C:212:MET:CE	2:D:212:MET:HE2	2.49	0.43
2:C:249:THR:HG22	2:C:254:LEU:HD12	2.00	0.43
1:A:99:VAL:O	1:A:127:VAL:HG23	2.18	0.43
1:B:47:ALA:HB3	1:B:99:VAL:HG22	2.01	0.43
2:D:50:LYS:HE3	2:D:79:ASP:HB2	1.99	0.43
2:C:151:PHE:CD2	2:C:151:PHE:N	2.87	0.42
1:A:142:LEU:HD13	1:A:143:TYR:CE1	2.54	0.42
1:B:25:SER:O	1:B:26:LEU:HD23	2.19	0.42
2:C:121:ALA:HB1	2:C:149:PRO:HD3	2.01	0.42
1:B:251:THR:OG1	1:B:266:GLN:HG2	2.18	0.42
2:C:264:GLN:HA	2:C:264:GLN:OE1	2.20	0.42
2:D:219:TRP:CZ2	2:D:262:ILE:HD11	2.54	0.42
1:B:12:LEU:CD1	1:B:77:ILE:HG13	2.46	0.42
2:C:183:ARG:NH1	2:D:184:GLU:OE1	2.53	0.42
2:D:258:LEU:HD21	2:D:288:LEU:HD13	2.01	0.42
2:D:216:VAL:N	2:D:229:ASN:ND2	2.41	0.42
2:C:18:THR:HG22	2:C:22:ARG:NH1	2.35	0.42
1:A:52:GLY:HA3	3:A:401:GOL:O1	2.19	0.41
1:B:63:TYR:O	1:B:68:MET:HB3	2.20	0.41
2:C:202:LEU:HA	2:C:202:LEU:HD23	1.90	0.41
2:D:248:ILE:HA	2:D:248:ILE:HD12	1.84	0.41
2:C:201:HIS:CD2	2:D:202:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:HA	1:A:353:ASN:OD1	2.20	0.41
2:D:152:ASP:HB3	2:D:156:ARG:H	1.86	0.41
1:A:56:HIS:CE1	1:A:217:ILE:HD12	2.55	0.41
1:B:199:ALA:O	1:B:201:LYS:HE2	2.20	0.41
1:B:114:GLU:HG2	1:B:262:TRP:CH2	2.56	0.41
1:A:3:LYS:HB3	1:A:5:ILE:HG12	2.01	0.41
2:C:205:LEU:HD23	2:D:205:LEU:HB3	2.03	0.41
2:C:144:ALA:CB	2:C:170:THR:HG23	2.51	0.41
2:D:91:PRO:O	2:D:95:GLN:CG	2.69	0.41
1:A:48:LEU:HD22	1:A:161:GLY:HA2	2.03	0.41
2:C:73:CYS:HA	2:C:93:THR:HG21	2.02	0.41
2:C:288:LEU:HA	2:C:300:ILE:O	2.21	0.41
1:B:254:PHE:CE2	1:B:263:GLN:HB3	2.56	0.41
1:B:7:ASP:CG	1:B:9:GLN:HE22	2.25	0.40
1:B:59:MET:HA	1:B:60:HIS:HA	1.80	0.40
2:C:76:PHE:CD1	2:C:87:ARG:HG2	2.56	0.40
2:C:35:PRO:HG2	2:C:106:THR:HG21	2.02	0.40
2:D:277:SER:C	2:D:278:GLN:HG3	2.42	0.40
2:D:268:LEU:O	2:D:287:THR:HA	2.21	0.40
1:B:10:ASP:O	1:B:11:VAL:C	2.59	0.40
2:D:246:ARG:HH11	2:D:246:ARG:HG2	1.87	0.40
1:B:191:LEU:CD2	1:B:211:MET:HB3	2.52	0.40
2:C:152:ASP:O	2:C:155:GLY:N	2.46	0.40
2:D:289:LYS:HA	2:D:290:PRO:HD2	2.00	0.40

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	354/356 (99%)	327 (92%)	24 (7%)	3 (1%)	24 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	354/356 (99%)	322 (91%)	30 (8%)	2 (1%)	30	72
2	C	293/318 (92%)	267 (91%)	19 (6%)	7 (2%)	7	41
2	D	293/318 (92%)	274 (94%)	14 (5%)	5 (2%)	11	50
All	All	1294/1348 (96%)	1190 (92%)	87 (7%)	17 (1%)	15	56

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	220	ASP
1	A	140	ASP
2	C	40	GLY
2	C	230	ALA
2	C	265	ALA
1	A	135	ASP
2	C	153	SER
2	C	242	ALA
2	D	240	ALA
2	C	15	LEU
2	D	278	GLN
1	B	140	ASP
1	A	150	VAL
2	D	27	MET
2	D	118	LEU
1	B	150	VAL
2	D	91	PRO

### 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	287/288 (100%)	264 (92%)	23 (8%)	15	50
1	B	287/288 (100%)	268 (93%)	19 (7%)	21	60
2	C	241/260 (93%)	203 (84%)	38 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	241/260 (93%)	197 (82%)	44 (18%)	2	10
All	All	1056/1096 (96%)	932 (88%)	124 (12%)	7	29

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	8	VAL
1	A	9	GLN
1	A	12	LEU
1	A	30	GLN
1	A	45	LYS
1	A	82	THR
1	A	91	MET
1	A	142	LEU
1	A	178	ARG
1	A	196	VAL
1	A	205	THR
1	A	209	ASN
1	A	247	SER
1	A	250	ARG
1	A	253	ARG
1	A	274	SER
1	A	291	SER
1	A	302	THR
1	A	305	GLN
1	A	310	THR
1	A	339	THR
1	A	356	LYS
1	B	2	LYS
1	B	3	LYS
1	B	9	GLN
1	B	12	LEU
1	B	33	VAL
1	B	82	THR
1	B	132	ILE
1	B	134	ASP
1	B	138	VAL
1	B	139	LYS
1	B	142	LEU
1	B	196	VAL
1	B	201	LYS

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Mol	Chain	Res	Type
1	B	233	GLN
1	B	237	GLU
1	B	250	ARG
1	B	258	GLN
1	B	306	GLN
1	B	356	LYS
2	C	24	ASN
2	C	26	LEU
2	C	33	ASN
2	C	34	VAL
2	C	42	THR
2	C	51	LYS
2	C	63	ASP
2	C	80	GLU
2	C	88	ASN
2	C	92	GLN
2	C	120	LEU
2	C	126	GLN
2	C	142	ASN
2	C	154	LYS
2	C	170	THR
2	C	188	LEU
2	C	191	THR
2	C	195	LEU
2	C	198	THR
2	C	201	HIS
2	C	205	LEU
2	C	211	SER
2	C	216	VAL
2	C	220	ASP
2	C	229	ASN
2	C	231	GLN
2	C	244	GLN
2	C	246	ARG
2	C	252	LEU
2	C	253	THR
2	C	258	LEU
2	C	266	HIS
2	C	269	LYS
2	C	272	GLU
2	C	285	VAL
2	C	293	GLU

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Mol	Chain	Res	Type
2	C	297	THR
2	C	300	ILE
2	D	21	GLU
2	D	34	VAL
2	D	42	THR
2	D	45	SER
2	D	51	LYS
2	D	75	LEU
2	D	80	GLU
2	D	87	ARG
2	D	88	ASN
2	D	91	PRO
2	D	95	GLN
2	D	120	LEU
2	D	142	ASN
2	D	150	LEU
2	D	153	SER
2	D	154	LYS
2	D	156	ARG
2	D	168	GLU
2	D	170	THR
2	D	188	LEU
2	D	190	LEU
2	D	191	THR
2	D	195	LEU
2	D	197	GLU
2	D	198	THR
2	D	200	ARG
2	D	202	LEU
2	D	208	LEU
2	D	212	MET
2	D	214	ASP
2	D	216	VAL
2	D	225	LEU
2	D	229	ASN
2	D	237	ARG
2	D	239	ASP
2	D	241	THR
2	D	252	LEU
2	D	253	THR
2	D	257	VAL
2	D	263	LYS

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Mol	Chain	Res	Type
2	D	278	GLN
2	D	282	ILE
2	D	285	VAL
2	D	300	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	183	GLN
1	A	185	HIS
1	A	209	ASN
1	A	249	HIS
1	A	314	ASN
1	B	9	GLN
1	B	29	HIS
1	B	30	GLN
1	B	183	GLN
1	B	185	HIS
1	B	305	GLN
2	C	88	ASN
2	C	201	HIS
2	C	206	ASN
2	C	226	GLN
2	C	229	ASN
2	C	278	GLN
2	D	58	GLN
2	D	201	HIS
2	D	229	ASN
2	D	295	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

2 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	GOL	A	401	-	5,5,5	0.40	0	5,5,5	0.58	0
3	GOL	B	401	-	5,5,5	0.25	0	5,5,5	0.56	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
3	GOL	A	401	-	-	0/4/4/4	0/0/0/0
3	GOL	B	401	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	6	0
3	B	401	GOL	5	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	356/356 (100%)	-0.31	1 (0%) 94 93	50, 66, 86, 96	0
1	B	356/356 (100%)	-0.30	0 100 100	47, 66, 86, 97	0
2	C	295/318 (92%)	-0.13	4 (1%) 78 69	41, 65, 107, 121	0
2	D	295/318 (92%)	-0.16	1 (0%) 94 93	44, 63, 100, 119	0
All	All	1302/1348 (96%)	-0.23	6 (0%) 91 88	41, 65, 94, 121	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	294	THR	3.1
2	C	292	ILE	3.1
2	C	296	GLY	2.7
2	D	294	THR	2.6
1	A	356	LYS	2.3
2	C	293	GLU	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	401	6/6	0.93	0.20	2.01	76,79,81,83	0
3	GOL	A	401	6/6	0.92	0.20	1.57	69,71,72,75	0

## 6.5 Other polymers

There are no such residues in this entry.