



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2025 – 06:16 AM EDT

PDB ID : 3HIJ  
Title : Crystal structure of dihydrodipicolinate synthase from *Bacillus anthracis* in complex with its substrate, pyruvate  
Authors : Voss, J.E.; Scally, S.W.; Dobson, R.C.J.; Perugini, M.A.  
Deposited on : 2009-05-20  
Resolution : 2.15 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

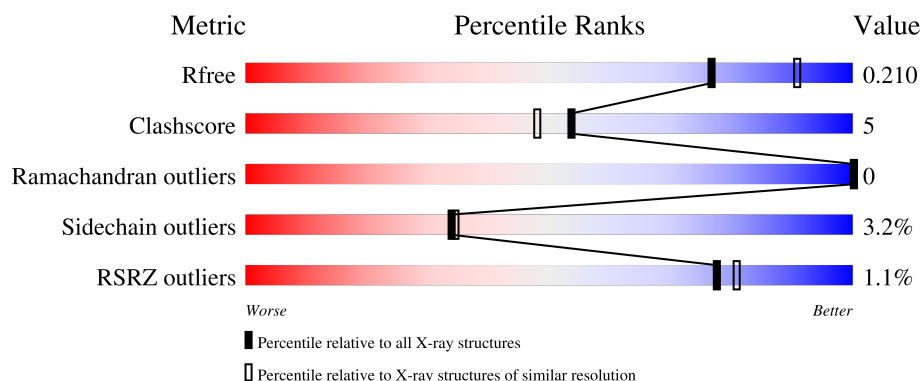
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
$R_{free}$	164625	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	292	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	B	292	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	292	<div> <div></div> <div> <div></div> <div>90%</div> <div>8%</div> <div>.</div> </div> </div>
1	D	292	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>.</div> </div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	294	-	-	X	-

## 2 Entry composition [i](#)

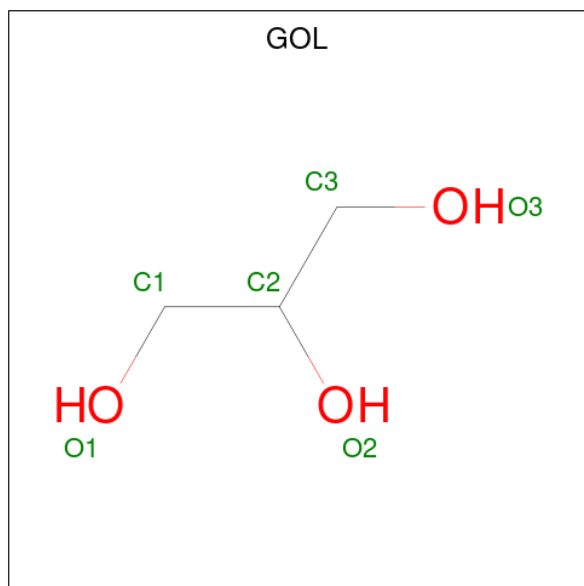
There are 4 unique types of molecules in this entry. The entry contains 9957 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2194	1391	361	430	12			
1	B	292	Total	C	N	O	S	0	0	0
			2194	1391	361	430	12			
1	C	292	Total	C	N	O	S	0	0	0
			2194	1391	361	430	12			
1	D	292	Total	C	N	O	S	0	0	0
			2194	1391	361	430	12			

- Molecule 2 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
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	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	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		

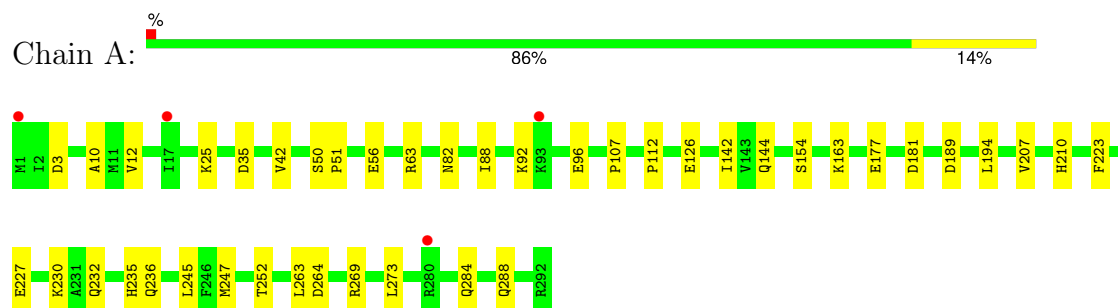
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	323	Total	O	0	0
			323	323		
4	B	302	Total	O	0	0
			302	302		
4	C	259	Total	O	0	0
			259	259		
4	D	269	Total	O	0	0
			269	269		

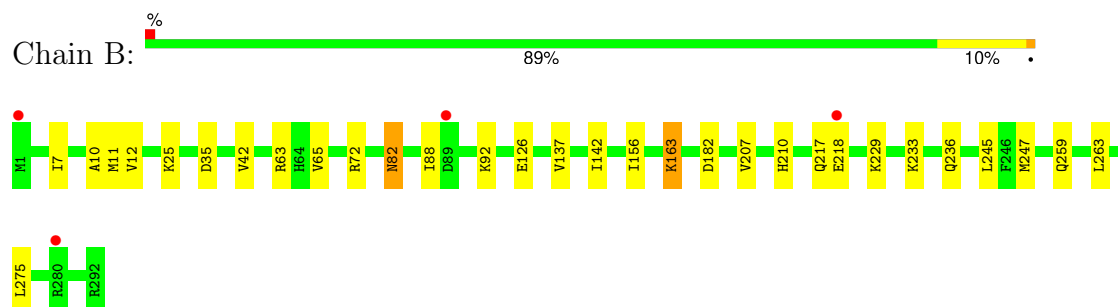
### 3 Residue-property plots [i](#)

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 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.

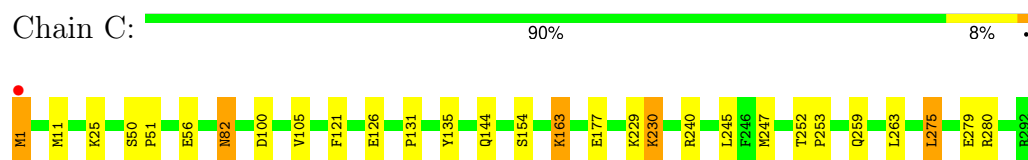
#### • Molecule 1: Dihydrodipicolinate synthase



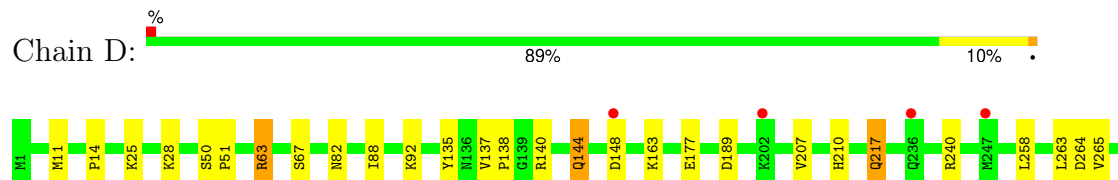
#### • Molecule 1: Dihydrodipicolinate synthase



#### • Molecule 1: Dihydrodipicolinate synthase



#### • Molecule 1: Dihydrodipicolinate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.48Å 124.62Å 130.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.27 – 2.15 37.27 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.27-2.15) 100.0 (37.27-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.64 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.153 , 0.210 0.153 , 0.210	Depositor DCC
$R_{free}$ test set	3066 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.5	Xtriage
Anisotropy	0.850	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9957	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: KPI, GOL, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.08	2/2213 (0.1%)	0.91	5/3011 (0.2%)
1	B	1.11	1/2213 (0.0%)	1.00	6/3011 (0.2%)
1	C	1.06	3/2213 (0.1%)	0.88	0/3011
1	D	1.05	1/2213 (0.0%)	0.87	2/3011 (0.1%)
All	All	1.08	7/8852 (0.1%)	0.92	13/12044 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	ARG	CZ-NH1	7.96	1.43	1.33
1	A	96	GLU	CG-CD	7.56	1.63	1.51
1	D	278	GLU	CG-CD	6.45	1.61	1.51
1	C	121	PHE	CD1-CE1	6.12	1.51	1.39
1	C	56	GLU	CB-CG	5.16	1.61	1.52
1	A	56	GLU	CG-CD	5.07	1.59	1.51
1	C	56	GLU	CG-CD	5.00	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ARG	NE-CZ-NH2	-13.49	113.56	120.30
1	B	63	ARG	NE-CZ-NH1	12.20	126.40	120.30
1	B	35	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	A	63	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	3	ASP	CB-CG-OD1	6.16	123.84	118.30
1	A	181	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	35	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	63	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	230	LYS	CD-CE-NZ	-5.48	99.09	111.70
1	D	140	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	182	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	72	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2194	0	2245	23	0
1	B	2194	0	2244	28	0
1	C	2194	0	2244	20	0
1	D	2194	0	2244	17	0
2	A	6	0	8	0	0
2	B	12	0	16	9	0
2	D	6	0	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	323	0	0	8	1
4	B	302	0	0	6	1
4	C	259	0	0	7	0
4	D	269	0	0	6	0
All	All	9957	0	9009	85	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (85) 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:217:GLN:HB2	2:B:294:GOL:H32	1.43	0.99
1:B:217:GLN:CB	2:B:294:GOL:H32	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLN:HG3	4:A:935:HOH:O	1.65	0.95
1:B:217:GLN:HB2	2:B:294:GOL:C3	1.99	0.91
1:D:92:LYS:HE2	4:D:1217:HOH:O	1.70	0.91
1:C:247:MET:HB2	4:C:940:HOH:O	1.71	0.90
1:B:247:MET:HB2	4:B:1224:HOH:O	1.72	0.89
1:B:233:LYS:HB2	4:B:646:HOH:O	1.75	0.86
1:D:25:LYS:HE2	1:D:264:ASP:O	1.88	0.74
1:D:148:ASP:OD1	4:D:951:HOH:O	2.07	0.72
1:C:154:SER:O	4:C:298:HOH:O	2.08	0.71
1:D:189:ASP:OD2	4:D:474:HOH:O	2.09	0.70
1:C:240:ARG:HH11	1:C:240:ARG:HG2	1.56	0.69
1:C:163:KPI:H1B	4:C:1222:HOH:O	1.92	0.69
1:A:25:LYS:HE2	1:A:264:ASP:O	1.93	0.68
1:D:207:VAL:O	1:D:210:HIS:HD2	1.76	0.68
1:A:247:MET:HB2	4:A:1204:HOH:O	1.92	0.68
1:C:230:LYS:HD2	4:C:710:HOH:O	1.94	0.68
1:B:217:GLN:HB3	2:B:294:GOL:H32	1.74	0.67
1:A:35:ASP:OD1	4:A:745:HOH:O	2.12	0.67
1:A:207:VAL:O	1:A:210:HIS:HD2	1.79	0.66
1:A:264:ASP:OD1	4:A:398:HOH:O	2.12	0.66
1:A:154:SER:O	4:A:320:HOH:O	2.12	0.65
1:C:126:GLU:OE1	4:C:360:HOH:O	2.15	0.65
1:A:177:GLU:O	4:A:393:HOH:O	2.15	0.65
1:C:259:GLN:OE1	1:C:280:ARG:NH2	2.30	0.65
1:A:126:GLU:HG3	4:A:1199:HOH:O	1.96	0.64
1:C:1:MET:HB3	4:C:515:HOH:O	2.02	0.60
1:B:207:VAL:O	1:B:210:HIS:HD2	1.84	0.60
1:B:88:ILE:O	1:B:92:LYS:HG2	2.05	0.57
1:A:194:LEU:HD22	1:A:235:HIS:HB2	1.87	0.56
1:B:217:GLN:HB2	2:B:294:GOL:H31	1.85	0.56
1:A:236:GLN:OE1	1:D:177:GLU:HB2	2.05	0.56
1:D:14:PRO:HA	1:D:265:VAL:O	2.06	0.55
1:C:240:ARG:HG2	1:C:240:ARG:NH1	2.21	0.55
1:B:126:GLU:HG3	4:B:364:HOH:O	2.08	0.54
1:B:12:VAL:H	1:B:210:HIS:CE1	2.27	0.52
1:B:12:VAL:H	1:B:210:HIS:HE1	1.57	0.52
1:B:92:LYS:HE2	4:B:972:HOH:O	2.10	0.52
1:B:236:GLN:NE2	1:C:177:GLU:HG3	2.26	0.50
1:B:218:GLU:CG	2:B:294:GOL:H12	2.42	0.50
1:C:82:ASN:HD22	1:C:82:ASN:N	2.10	0.50
1:D:138:PRO:HG3	1:D:144:GLN:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:O	1:A:92:LYS:HG2	2.13	0.49
1:D:88:ILE:O	1:D:92:LYS:HG2	2.12	0.49
1:D:210:HIS:HB3	1:D:258:LEU:HD21	1.94	0.49
1:C:105:VAL:HA	1:C:135:TYR:HB3	1.95	0.48
1:D:217:GLN:HE21	1:D:217:GLN:HA	1.78	0.48
1:A:12:VAL:H	1:A:210:HIS:CE1	2.31	0.47
1:B:156:ILE:O	4:B:300:HOH:O	2.20	0.47
1:A:12:VAL:H	1:A:210:HIS:HE1	1.62	0.47
1:C:82:ASN:HD22	1:C:82:ASN:H	1.63	0.47
1:B:82:ASN:HD22	1:B:82:ASN:H	1.63	0.46
1:C:252:THR:HG22	1:C:275:LEU:HD13	1.96	0.46
1:D:207:VAL:O	1:D:210:HIS:CD2	2.63	0.46
1:B:163:KPI:H1B	4:B:1099:HOH:O	2.15	0.46
1:B:10:ALA:HA	1:B:42:VAL:HB	1.97	0.46
1:C:1:MET:HE1	4:C:1075:HOH:O	2.14	0.46
1:B:7:ILE:HD12	1:B:217:GLN:HG2	1.98	0.45
1:B:218:GLU:HG3	2:B:294:GOL:H12	1.97	0.45
1:A:194:LEU:HA	1:A:194:LEU:HD12	1.83	0.45
1:B:82:ASN:HD22	1:B:82:ASN:N	2.13	0.44
1:D:135:TYR:CE1	1:D:137:VAL:HB	2.52	0.44
1:A:107:PRO:HB2	1:A:112:PRO:HG3	1.99	0.44
1:B:137:VAL:HG13	1:B:137:VAL:O	2.17	0.44
1:A:10:ALA:HA	1:A:42:VAL:HB	1.99	0.44
1:A:189:ASP:OD2	4:A:581:HOH:O	2.21	0.44
1:B:11:MET:HE1	1:B:65:VAL:HG21	2.00	0.43
1:B:218:GLU:N	2:B:294:GOL:H12	2.32	0.43
1:C:50:SER:N	1:C:51:PRO:CD	2.81	0.43
1:C:82:ASN:H	1:C:82:ASN:ND2	2.15	0.43
1:D:285:SER:HB2	4:D:1111:HOH:O	2.19	0.43
1:A:142:ILE:HG12	1:B:142:ILE:CD1	2.49	0.42
1:C:275:LEU:HG	1:C:279:GLU:HB3	2.01	0.42
1:C:100:ASP:O	1:C:131:PRO:HD2	2.20	0.42
1:A:252:THR:HG21	1:A:273:LEU:O	2.20	0.42
1:D:63:ARG:NH1	4:D:962:HOH:O	2.46	0.41
1:A:232:GLN:O	1:A:236:GLN:HG2	2.20	0.41
1:B:218:GLU:CA	2:B:294:GOL:H12	2.50	0.41
1:D:50:SER:OG	1:D:51:PRO:HD3	2.21	0.41
1:B:25:LYS:HD3	1:B:25:LYS:HA	1.81	0.41
1:A:50:SER:N	1:A:51:PRO:CD	2.85	0.40
1:A:194:LEU:HD11	1:A:223:PHE:HB2	2.03	0.40
1:C:252:THR:HB	1:C:253:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:ARG:NE	4:D:913:HOH:O	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:478:HOH:O	4:B:756:HOH:O[3_555]	2.08	0.12

## 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	289/292 (99%)	282 (98%)	7 (2%)	0	100	100
1	B	289/292 (99%)	280 (97%)	9 (3%)	0	100	100
1	C	289/292 (99%)	280 (97%)	9 (3%)	0	100	100
1	D	289/292 (99%)	281 (97%)	8 (3%)	0	100	100
All	All	1156/1168 (99%)	1123 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	238 (98%)	6 (2%)	42	45
1	B	244/244 (100%)	238 (98%)	6 (2%)	42	45
1	C	244/244 (100%)	234 (96%)	10 (4%)	26	25
1	D	244/244 (100%)	235 (96%)	9 (4%)	29	28
All	All	976/976 (100%)	945 (97%)	31 (3%)	34	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	144	GLN
1	A	227	GLU
1	A	245	LEU
1	A	263	LEU
1	A	284	GLN
1	B	82	ASN
1	B	229	LYS
1	B	245	LEU
1	B	259	GLN
1	B	263	LEU
1	B	275	LEU
1	C	1	MET
1	C	11	MET
1	C	25	LYS
1	C	82	ASN
1	C	144	GLN
1	C	229	LYS
1	C	230	LYS
1	C	245	LEU
1	C	263	LEU
1	C	275	LEU
1	D	11	MET
1	D	28	LYS
1	D	67	SER
1	D	82	ASN
1	D	144	GLN
1	D	217	GLN
1	D	240	ARG
1	D	263	LEU
1	D	288	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	82	ASN
1	A	210	HIS
1	B	82	ASN
1	B	210	HIS
1	B	224	GLN
1	B	236	GLN
1	B	259	GLN
1	C	82	ASN
1	C	236	GLN
1	C	288	GLN
1	D	82	ASN
1	D	210	HIS
1	D	217	GLN
1	D	288	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	KPI	A	163	1	11,13,14	1.15	0	9,15,17	1.70	2 (22%)
1	KPI	B	163	1	11,13,14	1.02	0	9,15,17	2.13	4 (44%)
1	KPI	D	163	1	11,13,14	1.06	1 (9%)	9,15,17	1.93	3 (33%)
1	KPI	C	163	1	11,13,14	1.15	0	9,15,17	2.01	4 (44%)

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
1	KPI	A	163	1	-	1/13/14/16	-
1	KPI	B	163	1	-	0/13/14/16	-
1	KPI	D	163	1	-	0/13/14/16	-
1	KPI	C	163	1	-	1/13/14/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	KPI	O2-CX2	2.34	1.28	1.22

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	KPI	CD-CE-NZ	-4.02	103.55	110.67
1	B	163	KPI	CX2-CX1-NZ	3.42	122.93	114.88
1	A	163	KPI	CE-NZ-CX1	3.21	130.40	121.58
1	D	163	KPI	CD-CE-NZ	-3.12	105.14	110.67
1	D	163	KPI	CE-NZ-CX1	3.07	130.02	121.58
1	C	163	KPI	CE-NZ-CX1	2.99	129.80	121.58
1	C	163	KPI	CX2-CX1-NZ	2.33	120.36	114.88
1	C	163	KPI	O1-CX2-CX1	2.26	121.31	116.50
1	D	163	KPI	CX2-CX1-NZ	2.24	120.16	114.88
1	A	163	KPI	CD-CG-CB	-2.13	105.59	113.62
1	B	163	KPI	CD-CG-CB	-2.09	105.74	113.62
1	C	163	KPI	O2-CX2-CX1	-2.08	118.80	121.35
1	B	163	KPI	CE-NZ-CX1	2.05	127.21	121.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	163	KPI	O-C-CA-CB
1	C	163	KPI	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	163	KPI	1	0

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*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	163	KPI	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	293	-	5,5,5	0.48	0	5,5,5	0.81	0
2	GOL	B	293	-	5,5,5	0.43	0	5,5,5	0.48	0
2	GOL	A	293	-	5,5,5	0.44	0	5,5,5	0.40	0
2	GOL	B	294	-	5,5,5	0.56	0	5,5,5	1.00	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	D	293	-	-	3/4/4/4	-
2	GOL	B	293	-	-	4/4/4/4	-
2	GOL	A	293	-	-	4/4/4/4	-
2	GOL	B	294	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	293	GOL	C1-C2-C3-O3
2	B	293	GOL	O1-C1-C2-C3
2	B	294	GOL	C1-C2-C3-O3
2	B	293	GOL	O2-C2-C3-O3
2	A	293	GOL	O1-C1-C2-C3
2	B	293	GOL	C1-C2-C3-O3
2	D	293	GOL	O1-C1-C2-C3
2	D	293	GOL	C1-C2-C3-O3
2	A	293	GOL	O2-C2-C3-O3
2	B	293	GOL	O1-C1-C2-O2
2	B	294	GOL	O2-C2-C3-O3
2	D	293	GOL	O1-C1-C2-O2
2	A	293	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	294	GOL	9	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	291/292 (99%)	-0.84	4 (1%) 73 77	3, 14, 28, 47	6 (2%)
1	B	291/292 (99%)	-0.80	4 (1%) 73 77	3, 14, 29, 45	7 (2%)
1	C	291/292 (99%)	-0.81	1 (0%) 90 92	7, 16, 30, 50	4 (1%)
1	D	291/292 (99%)	-0.68	4 (1%) 73 77	6, 18, 31, 45	6 (2%)
All	All	1164/1168 (99%)	-0.78	13 (1%) 77 81	3, 16, 30, 50	23 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	ARG	4.5
1	A	93	LYS	4.2
1	B	1	MET	4.2
1	D	148	ASP	4.1
1	B	218	GLU	3.8
1	A	17	ILE	3.7
1	D	236	GLN	3.4
1	D	247	MET	3.4
1	A	280	ARG	3.1
1	B	89	ASP	2.9
1	C	1	MET	2.8
1	A	1	MET	2.5
1	D	202	LYS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	KPI	C	163	14/15	0.96	0.06	13,15,22,24	0
1	KPI	D	163	14/15	0.96	0.06	11,14,23,24	0
1	KPI	B	163	14/15	0.97	0.05	9,13,19,20	0
1	KPI	A	163	14/15	0.98	0.04	10,11,17,18	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	293	6/6	0.78	0.17	48,53,55,57	0
2	GOL	A	293	6/6	0.79	0.16	61,63,64,64	0
2	GOL	D	293	6/6	0.82	0.15	42,48,49,50	0
2	GOL	B	294	6/6	0.86	0.19	44,50,52,53	0
3	NA	B	295	1/1	0.95	0.04	24,24,24,24	0
3	NA	A	294	1/1	0.99	0.05	20,20,20,20	0
3	NA	C	293	1/1	0.99	0.02	23,23,23,23	0
3	NA	D	294	1/1	0.99	0.08	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.