



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:51 PM GMT

PDB ID : 3A3D  
Title : Crystal structure of penicillin binding protein 4 (dacB) from Haemophilus influenzae  
Authors : Kawai, F.; Roper, D.I.; Park, S.-Y.; Tame, J.R.H.  
Deposited on : 2009-06-12  
Resolution : 1.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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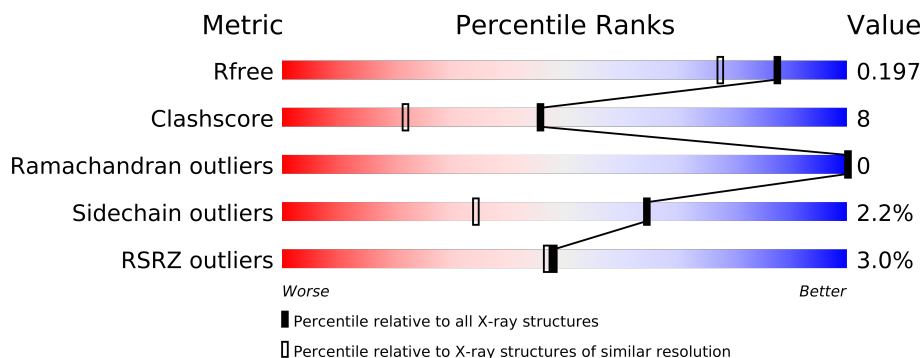
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	453	
1	B	453	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	GOL	A	480	-	X
2	GOL	A	481	-	X
2	GOL	A	482	-	X

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7960 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.

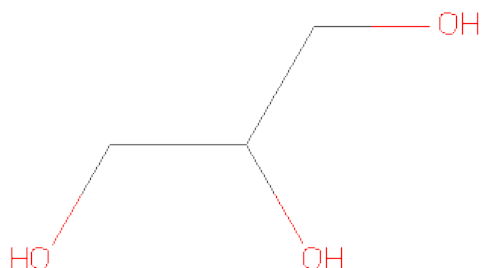
- Molecule 1 is a protein called Penicillin-binding protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3506	2237	605	652	12			
1	B	453	Total	C	N	O	S	4	0	0
			3506	2237	605	652	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	EXPRESSION TAG	UNP A8E0K8
B	27	MET	-	EXPRESSION TAG	UNP A8E0K8

- 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		

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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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

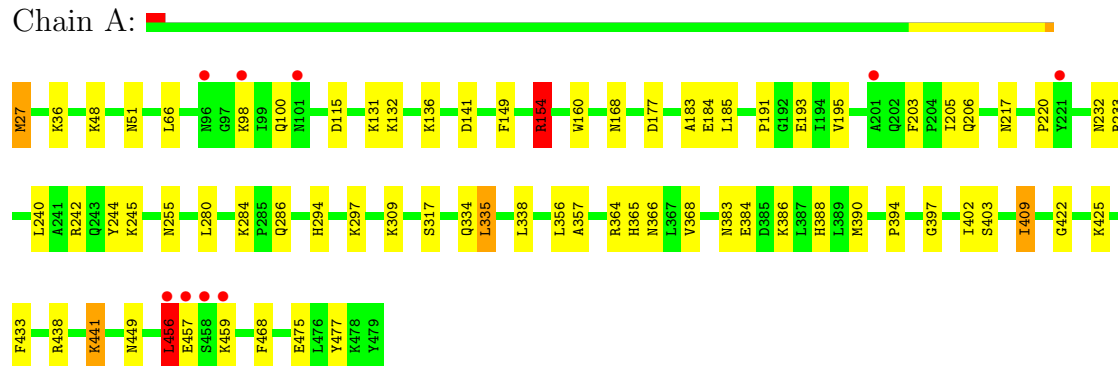
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	512	Total	O	0	0
			512	512		
3	B	412	Total	O	0	0
			412	412		

### 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.

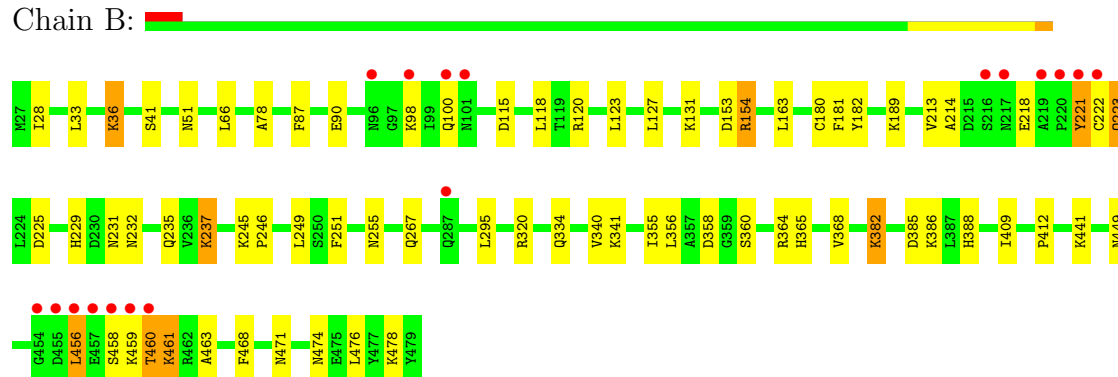
- Molecule 1: Penicillin-binding protein 4

Chain A:



- Molecule 1: Penicillin-binding protein 4

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.55Å 92.59Å 104.88Å 90.00° 107.75° 90.00°	Depositor
Resolution (Å)	19.98 – 1.60 19.98 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-1.60) 94.9 (19.98-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.02 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.171 , 0.204 0.165 , 0.197	Depositor DCC
$R_{free}$ test set	7346 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.1	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 146602 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	1.42	11/3572 (0.3%)	1.30	19/4830 (0.4%)
1	B	1.36	6/3572 (0.2%)	1.28	17/4830 (0.4%)
All	All	1.39	17/7144 (0.2%)	1.29	36/9660 (0.4%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ALA	CA-CB	-7.95	1.35	1.52
1	B	182	TYR	CD1-CE1	6.86	1.49	1.39
1	B	320	ARG	CZ-NH1	6.63	1.41	1.33
1	B	360	SER	CB-OG	6.00	1.50	1.42
1	A	203	PHE	CE1-CZ	5.88	1.48	1.37
1	A	368	VAL	CB-CG1	-5.65	1.41	1.52
1	A	477	TYR	CG-CD1	-5.61	1.31	1.39
1	A	160	TRP	CG-CD1	5.54	1.44	1.36
1	B	87	PHE	CD1-CE1	5.51	1.50	1.39
1	A	149	PHE	CE1-CZ	5.50	1.47	1.37
1	A	477	TYR	CD1-CE1	5.40	1.47	1.39
1	B	78	ALA	CA-CB	5.26	1.63	1.52
1	A	468	PHE	CE1-CZ	5.13	1.47	1.37
1	A	475	GLU	CD-OE2	-5.12	1.20	1.25
1	B	41	SER	CA-CB	5.12	1.60	1.52
1	A	184	GLU	CD-OE2	5.11	1.31	1.25
1	A	456	LEU	CG-CD1	5.06	1.70	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ARG	NE-CZ-NH2	-15.77	112.41	120.30
1	A	242	ARG	NE-CZ-NH1	10.67	125.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	LEU	CB-CG-CD1	9.27	126.76	111.00
1	B	320	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	B	127	LEU	CB-CG-CD1	-7.66	97.98	111.00
1	A	27	MET	CB-CG-SD	-7.61	89.56	112.40
1	B	456	LEU	CA-CB-CG	7.40	132.32	115.30
1	A	433	PHE	CB-CG-CD2	-7.33	115.67	120.80
1	A	154	ARG	CB-CG-CD	6.79	129.26	111.60
1	B	356	LEU	CB-CG-CD2	-6.57	99.84	111.00
1	B	115	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	335	LEU	CB-CG-CD2	-6.25	100.38	111.00
1	A	280	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	A	364	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	131	LYS	CB-CG-CD	-5.88	96.33	111.60
1	B	118	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	B	115	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	317	SER	CB-CA-C	-5.75	99.18	110.10
1	A	297	LYS	CD-CE-NZ	-5.66	98.69	111.70
1	A	356	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	A	115	ASP	CB-CG-OD1	5.64	123.37	118.30
1	B	364	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	48	LYS	CD-CE-NZ	-5.60	98.82	111.70
1	B	358	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	154	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	154	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	177	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	B	221	TYR	CB-CA-C	-5.38	99.64	110.40
1	A	438	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	A	441	LYS	CD-CE-NZ	-5.22	99.70	111.70
1	B	237	LYS	CD-CE-NZ	-5.18	99.79	111.70
1	B	123	LEU	CB-CG-CD1	5.17	119.79	111.00
1	B	225	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	B	153	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	340	VAL	CA-CB-CG2	-5.07	103.29	110.90
1	A	422	GLY	N-CA-C	-5.06	100.44	113.10

There are no chirality outliers.

There are no planarity outliers.

## 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	3506	0	3554	63	0
1	B	3506	0	3554	56	0
2	A	18	0	24	6	0
2	B	6	0	8	3	0
3	A	512	0	0	22	0
3	B	412	0	0	18	0
All	All	7960	0	7140	117	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 8.

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:335:LEU:HD12	3:A:877:HOH:O	1.22	1.32
1:A:441:LYS:HE2	2:A:482:GOL:O1	1.29	1.28
1:A:141:ASP:OD1	2:A:480:GOL:H11	1.46	1.14
1:B:98:LYS:HE2	1:B:100:GLN:CD	1.71	1.09
1:A:441:LYS:HE2	2:A:482:GOL:HO1	1.21	0.95
1:B:66:LEU:H	1:B:449:ASN:HD21	1.13	0.95
1:A:66:LEU:H	1:A:449:ASN:HD21	1.13	0.94
1:A:456:LEU:H	1:A:456:LEU:CD1	1.81	0.93
1:A:232:ASN:HD21	1:A:255:ASN:H	1.16	0.90
1:A:441:LYS:CE	2:A:482:GOL:O1	2.20	0.87
1:A:456:LEU:HD12	1:A:456:LEU:H	1.38	0.86
1:B:368:VAL:HG23	3:B:835:HOH:O	1.75	0.86
1:B:98:LYS:HE2	1:B:100:GLN:NE2	1.92	0.83
1:A:193:GLU:HG3	3:A:829:HOH:O	1.79	0.83
1:B:460:THR:HG23	3:B:708:HOH:O	1.79	0.83
1:A:98:LYS:NZ	1:A:100:GLN:OE1	2.14	0.81
1:B:232:ASN:HD21	1:B:255:ASN:H	1.29	0.80
1:B:154:ARG:HD3	3:B:669:HOH:O	1.81	0.79
1:B:36:LYS:HD3	1:B:468:PHE:HA	1.65	0.77
1:B:33:LEU:O	1:B:36:LYS:HD2	1.86	0.76
1:B:267:GLN:HE21	2:B:1:GOL:H32	1.51	0.76
1:B:368:VAL:CG2	3:B:835:HOH:O	2.33	0.75
1:A:98:LYS:HB2	1:A:98:LYS:NZ	2.01	0.75
1:A:357:ALA:H	1:A:366:ASN:ND2	1.84	0.74
1:A:335:LEU:CD1	3:A:877:HOH:O	1.97	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:LEU:HD13	3:A:936:HOH:O	1.91	0.71
1:A:98:LYS:HB2	1:A:98:LYS:HZ2	1.56	0.70
1:B:131:LYS:HE3	3:B:808:HOH:O	1.91	0.69
1:B:36:LYS:NZ	1:B:471:ASN:HD22	1.92	0.67
1:B:154:ARG:HD2	1:B:163:LEU:HD22	1.76	0.66
1:A:244:TYR:C	1:A:245:LYS:HG3	2.14	0.65
1:B:461:LYS:HD2	1:B:463:ALA:H	1.61	0.64
1:A:357:ALA:H	1:A:366:ASN:HD21	1.44	0.63
1:A:232:ASN:ND2	1:A:255:ASN:H	1.93	0.63
1:A:66:LEU:H	1:A:449:ASN:ND2	1.93	0.62
1:B:232:ASN:ND2	1:B:255:ASN:H	1.98	0.62
1:A:141:ASP:CG	2:A:480:GOL:H11	2.18	0.62
1:B:66:LEU:H	1:B:449:ASN:ND2	1.93	0.61
1:A:309:LYS:NZ	3:A:648:HOH:O	2.34	0.60
1:B:51:ASN:ND2	1:B:441:LYS:H	1.99	0.60
1:A:51:ASN:ND2	1:A:441:LYS:H	1.99	0.60
1:A:98:LYS:CB	1:A:98:LYS:NZ	2.65	0.60
1:B:98:LYS:HE2	1:B:100:GLN:OE1	2.03	0.59
1:B:36:LYS:HD3	1:B:468:PHE:CA	2.33	0.59
1:A:284:LYS:HG3	1:A:286:GLN:NE2	2.20	0.57
1:B:341:LYS:CE	3:B:859:HOH:O	2.52	0.57
1:B:36:LYS:HZ1	1:B:471:ASN:HD22	1.51	0.57
1:B:386:LYS:HG2	3:B:585:HOH:O	2.05	0.56
1:B:66:LEU:N	1:B:449:ASN:HD21	1.93	0.56
1:A:425:LYS:NZ	1:A:456:LEU:HB3	2.20	0.56
1:A:456:LEU:HD12	1:A:456:LEU:N	2.15	0.55
1:A:141:ASP:OD1	2:A:480:GOL:C1	2.36	0.55
1:A:334:GLN:NE2	1:B:223:GLN:OE1	2.41	0.54
1:A:98:LYS:CE	1:A:100:GLN:OE1	2.56	0.54
1:B:388:HIS:HE1	3:B:769:HOH:O	1.91	0.53
1:A:245:LYS:HE2	3:A:975:HOH:O	2.07	0.53
1:A:193:GLU:HG3	3:A:901:HOH:O	2.09	0.53
1:A:233:ARG:HD3	3:A:674:HOH:O	2.09	0.52
3:A:531:HOH:O	1:B:365:HIS:HE1	1.93	0.51
1:A:132:LYS:NZ	3:A:886:HOH:O	2.43	0.51
1:A:397:GLY:HA2	1:A:403:SER:O	2.11	0.50
3:A:548:HOH:O	1:B:334:GLN:HG3	2.10	0.50
1:B:120:ARG:HE	2:B:1:GOL:C2	2.24	0.50
1:A:338:LEU:HG	3:A:860:HOH:O	2.12	0.49
1:A:168:ASN:ND2	3:A:757:HOH:O	2.26	0.49
1:A:244:TYR:O	1:A:245:LYS:HG3	2.11	0.49
1:A:240:LEU:N	1:A:240:LEU:HD23	2.26	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:180:CYS:SG	3:B:509:HOH:O	2.60	0.49
1:A:425:LYS:HZ1	1:A:456:LEU:HB3	1.75	0.49
1:A:386:LYS:HE3	3:A:806:HOH:O	2.13	0.48
1:B:51:ASN:HD21	1:B:441:LYS:H	1.59	0.48
1:A:294:HIS:HE1	3:A:4:HOH:O	1.96	0.48
1:A:206:GLN:OE1	3:A:910:HOH:O	2.20	0.48
1:B:237:LYS:HE2	3:B:704:HOH:O	2.12	0.48
1:A:456:LEU:HD11	3:B:724:HOH:O	2.14	0.47
1:A:66:LEU:N	1:A:449:ASN:HD21	1.97	0.47
1:B:231:ASN:ND2	3:B:888:HOH:O	2.48	0.46
1:A:456:LEU:HG	1:B:355:ILE:HD12	1.97	0.46
1:A:456:LEU:HD22	3:B:749:HOH:O	2.16	0.45
1:B:478:LYS:HE2	1:B:478:LYS:HB2	1.56	0.45
1:A:154:ARG:CD	3:A:825:HOH:O	2.64	0.45
1:A:394:PRO:HB2	1:A:402:ILE:HG12	1.98	0.45
1:B:267:GLN:NE2	2:B:1:GOL:H32	2.24	0.45
1:A:388:HIS:HE1	3:A:960:HOH:O	1.99	0.45
1:B:218:GLU:O	1:B:221:TYR:HB2	2.16	0.45
1:A:51:ASN:H	1:A:51:ASN:HD22	1.65	0.45
1:A:384:GLU:OE1	1:A:390:MET:HG2	2.17	0.45
1:A:284:LYS:NZ	1:A:286:GLN:HE22	2.15	0.44
1:B:341:LYS:HE2	3:B:698:HOH:O	2.17	0.44
1:B:385:ASP:HB3	3:B:585:HOH:O	2.17	0.44
1:B:90:GLU:HG2	1:B:295:LEU:CD2	2.48	0.43
1:B:412:PRO:HD2	1:B:474:ASN:HD21	1.82	0.43
1:B:249:LEU:HA	1:B:249:LEU:HD23	1.79	0.43
1:B:223:GLN:NE2	3:B:771:HOH:O	2.52	0.42
3:A:548:HOH:O	1:B:334:GLN:CG	2.67	0.42
1:A:383:ASN:HD22	1:A:386:LYS:NZ	2.17	0.42
1:B:28:ILE:CD1	1:B:476:LEU:HD23	2.49	0.42
1:B:51:ASN:HD22	1:B:51:ASN:H	1.67	0.42
1:A:205:ILE:C	1:A:205:ILE:HD12	2.40	0.42
1:A:154:ARG:HD3	3:A:825:HOH:O	2.18	0.42
1:A:365:HIS:HE1	3:B:613:HOH:O	2.02	0.42
1:B:382:LYS:HE3	1:B:382:LYS:HB2	1.88	0.41
1:B:229:HIS:HE1	1:B:235:GLN:OE1	2.03	0.41
1:B:214:ALA:CB	1:B:222:CYS:SG	3.08	0.41
1:B:461:LYS:HA	1:B:461:LYS:HD3	1.21	0.41
1:A:334:GLN:HG2	3:B:923:HOH:O	2.21	0.41
1:B:245:LYS:HA	1:B:246:PRO:HD2	1.85	0.41
1:A:409:ILE:CD1	1:A:409:ILE:C	2.88	0.41
1:A:185:LEU:HB3	1:A:195:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:217:ASN:O	1:A:220:PRO:HD2	2.21	0.41
1:B:98:LYS:CE	1:B:100:GLN:NE2	2.74	0.40
1:A:284:LYS:HG3	1:A:286:GLN:HE21	1.86	0.40
3:A:826:HOH:O	1:B:456:LEU:HD13	2.20	0.40
1:B:189:LYS:HB2	1:B:213:VAL:HG21	2.03	0.40
1:A:193:GLU:CG	3:A:829:HOH:O	2.53	0.40
1:B:214:ALA:HB2	1:B:222:CYS:SG	2.61	0.40
1:B:181:PHE:CZ	1:B:251:PHE:HB2	2.57	0.40

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	451/453 (100%)	442 (98%)	9 (2%)	0	100	100
1	B	451/453 (100%)	441 (98%)	10 (2%)	0	100	100
All	All	902/906 (100%)	883 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	378/378 (100%)	369 (98%)	9 (2%)	61	31
1	B	378/378 (100%)	370 (98%)	8 (2%)	66	37
All	All	756/756 (100%)	739 (98%)	17 (2%)	64	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	MET
1	A	36	LYS
1	A	136	LYS
1	A	154	ARG
1	A	191	PRO
1	A	409	ILE
1	A	456	LEU
1	A	457	GLU
1	A	459	LYS
1	B	36	LYS
1	B	223	GLN
1	B	382	LYS
1	B	409	ILE
1	B	458	SER
1	B	459	LYS
1	B	460	THR
1	B	461	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	51	ASN
1	A	232	ASN
1	A	283	GLN
1	A	286	GLN
1	A	294	HIS
1	A	325	ASN
1	A	345	GLN
1	A	365	HIS
1	A	366	ASN
1	A	383	ASN
1	A	388	HIS
1	A	449	ASN
1	B	51	ASN
1	B	103	ASN
1	B	139	ASN
1	B	179	ASN
1	B	198	ASN
1	B	217	ASN
1	B	229	HIS

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Mol	Chain	Res	Type
1	B	232	ASN
1	B	267	GLN
1	B	286	GLN
1	B	325	ASN
1	B	365	HIS
1	B	388	HIS
1	B	446	GLN
1	B	449	ASN
1	B	467	GLN
1	B	471	ASN
1	B	474	ASN

### 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 ⓘ

4 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	480	-	5,5,5	0.42	0	5,5,5	0.55	0
2	GOL	A	481	-	5,5,5	1.05	0	5,5,5	0.94	0
2	GOL	A	482	-	5,5,5	0.49	0	5,5,5	1.14	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	1	-	5,5,5	0.79	0	5,5,5	1.24	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	A	480	-	-	0/4/4/4	0/0/0/0
2	GOL	A	481	-	-	0/4/4/4	0/0/0/0
2	GOL	A	482	-	-	0/4/4/4	0/0/0/0
2	GOL	B	1	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GOL	O2-C2-C1	-2.69	95.96	108.22
2	A	482	GOL	O1-C1-C2	-2.16	99.18	109.71

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 ⓘ

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	453/453 (100%)	-0.42	9 (1%) 62 62	7, 14, 30, 47	0
1	B	453/453 (100%)	-0.13	18 (3%) 36 35	10, 18, 40, 65	1 (0%)
All	All	906/906 (100%)	-0.28	27 (2%) 48 47	7, 16, 34, 65	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	9.0
1	B	458	SER	8.8
1	B	220	PRO	6.9
1	B	455	ASP	6.3
1	B	457	GLU	6.1
1	B	454	GLY	5.4
1	B	459	LYS	5.3
1	B	460	THR	4.9
1	B	221	TYR	4.8
1	B	216	SER	4.6
1	A	459	LYS	4.0
1	B	101	ASN	3.9
1	B	219	ALA	3.8
1	B	217	ASN	3.8
1	A	457	GLU	3.2
1	B	222	CYS	3.2
1	B	98	LYS	3.2
1	A	98	LYS	3.2
1	A	456	LEU	3.1
1	A	458	SER	3.1
1	B	100	GLN	3.1
1	B	287	GLN	2.7
1	A	96	ASN	2.4
1	A	221	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	96	ASN	2.4
1	A	101	ASN	2.2
1	A	201	ALA	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	480	6/6	0.26	5.67	50,51,52,53	0
2	GOL	A	482	6/6	0.12	3.02	20,29,35,45	0
2	GOL	A	481	6/6	0.10	2.46	19,23,28,28	0
2	GOL	B	1	6/6	0.12	1.68	34,39,44,44	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.