



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:12 PM BST

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 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

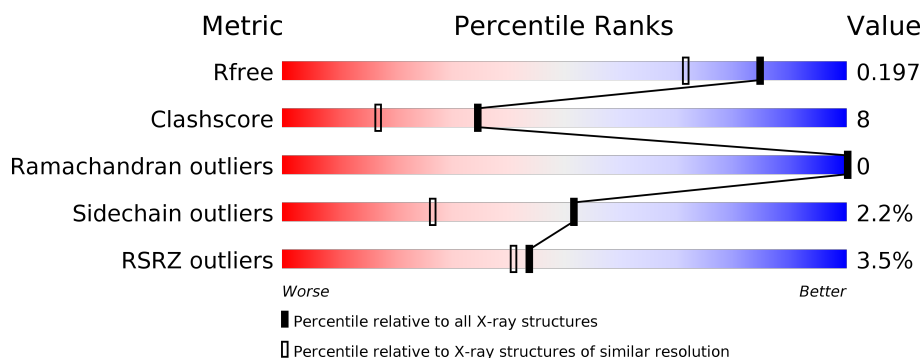
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 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	453	<div> <div>3%</div> <div>84%</div> <div>15%</div> </div>
1	B	453	<div> <div>4%</div> <div>84%</div> <div>14%</div> </div>

## 2 Entry composition [i](#)

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

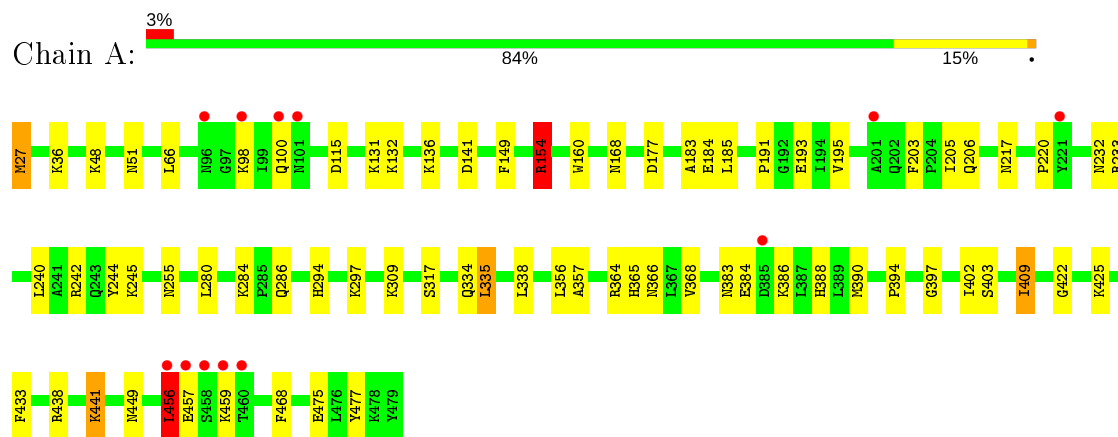
- Molecule 3 is water.

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

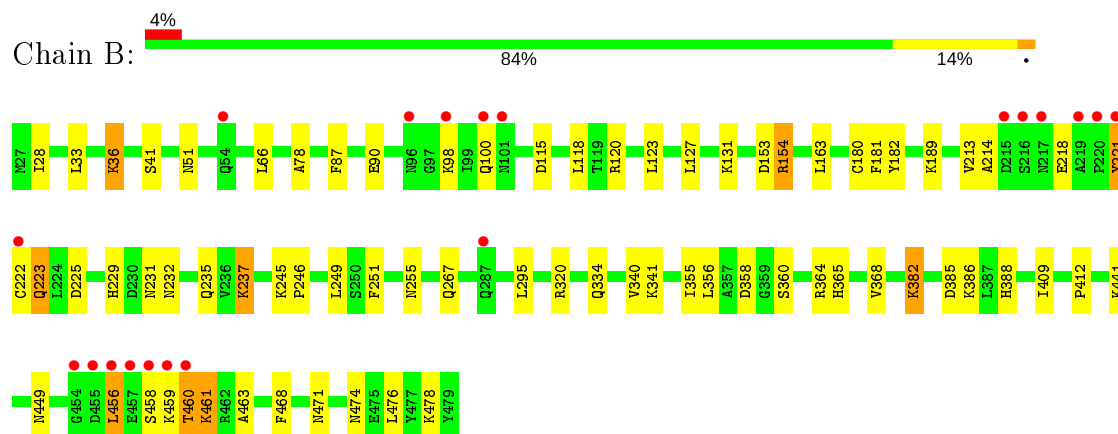
### 3 Residue-property plots [i](#)

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: Penicillin-binding protein 4



- Molecule 1: Penicillin-binding protein 4



## 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) 94.8 (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 (5.01%)	wwPDB-VP
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 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	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.

<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: 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 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	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

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 8.

All (117) 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: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:A:98:LYS:HB2	1:A:98:LYS:NZ	2.01	0.75
1:B:368:VAL:CG2	3:B:835:HOH:O	2.33	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	Interatomic distance (Å)	Clash overlap (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:168:ASN:ND2	3:A:757:HOH:O	2.26	0.49
1:A:338:LEU:HG	3:A:860:HOH:O	2.12	0.49
1:A:240:LEU:N	1:A:240:LEU:HD23	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:TYR:O	1:A:245:LYS:HG3	2.11	0.49
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:206:GLN:OE1	3:A:910:HOH:O	2.20	0.48
1:A:294:HIS:HE1	3:A:4:HOH:O	1.96	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:384:GLU:OE1	1:A:390:MET:HG2	2.17	0.45
1:A:51:ASN:H	1:A:51:ASN:HD22	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:181:PHE:CZ	1:B:251:PHE:HB2	2.57	0.40
1:B:214:ALA:HB2	1:B:222:CYS:SG	2.61	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	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 [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	378/378 (100%)	369 (98%)	9 (2%)	49	24
1	B	378/378 (100%)	370 (98%)	8 (2%)	53	29
All	All	756/756 (100%)	739 (98%)	17 (2%)	52	27

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

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Mol	Chain	Res	Type
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
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 [i](#)

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](#)

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	481	-	5,5,5	1.13	0	5,5,5	0.90	0
2	GOL	A	482	-	5,5,5	0.50	0	5,5,5	1.27	1 (20%)
2	GOL	A	480	-	5,5,5	0.41	0	5,5,5	0.61	0
2	GOL	B	1	-	5,5,5	0.77	0	5,5,5	1.38	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	481	-	-	0/4/4/4	-
2	GOL	A	482	-	-	0/4/4/4	-
2	GOL	A	480	-	-	4/4/4/4	-
2	GOL	B	1	-	-	3/4/4/4	-

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	-2.99	95.96	109.12
2	A	482	GOL	O1-C1-C2	-2.30	99.18	110.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	480	GOL	O1-C1-C2-C3
2	A	480	GOL	C1-C2-C3-O3
2	B	1	GOL	C1-C2-C3-O3
2	B	1	GOL	O1-C1-C2-C3
2	A	480	GOL	O1-C1-C2-O2
2	A	480	GOL	O2-C2-C3-O3
2	B	1	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	482	GOL	3	0
2	A	480	GOL	3	0
2	B	1	GOL	3	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 ⓘ

### 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%)	-0.36	12 (2%) 56 53	7, 14, 30, 47	0
1	B	453/453 (100%)	-0.07	20 (4%) 34 31	10, 18, 40, 65	1 (0%)
All	All	906/906 (100%)	-0.21	32 (3%) 44 41	7, 16, 34, 65	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	LEU	9.7
1	B	458	SER	9.2
1	B	455	ASP	7.1
1	B	220	PRO	7.0
1	B	457	GLU	6.8
1	B	459	LYS	6.1
1	B	454	GLY	6.0
1	B	460	THR	5.8
1	B	221	TYR	5.3
1	B	216	SER	4.9
1	A	459	LYS	4.6
1	B	222	CYS	4.2
1	B	217	ASN	4.1
1	B	101	ASN	3.8
1	A	457	GLU	3.7
1	B	219	ALA	3.6
1	B	98	LYS	3.6
1	B	100	GLN	3.5
1	A	458	SER	3.4
1	A	456	LEU	3.4
1	A	98	LYS	3.3
1	B	287	GLN	2.8
1	A	96	ASN	2.8
1	A	101	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	221	TYR	2.6
1	B	96	ASN	2.5
1	A	460	THR	2.5
1	A	201	ALA	2.4
1	A	100	GLN	2.3
1	B	215	ASP	2.2
1	B	54	GLN	2.0
1	A	385	ASP	2.0

## 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 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	A	480	6/6	0.74	0.25	50,51,52,53	0
2	GOL	A	482	6/6	0.87	0.12	20,29,35,45	0
2	GOL	B	1	6/6	0.89	0.12	34,39,44,44	0
2	GOL	A	481	6/6	0.91	0.10	19,23,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.