



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:16 pm BST

PDB ID : 6GWU  
Title : Carbonic anhydrase CaNce103p from *Candida albicans*  
Authors : Brynda, J.; Dostal, J.; Heidingsfeld, O.; Machacek, S.; Blaha, J.; Pichova, I.  
Deposited on : 2018-06-26  
Resolution : 2.20 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 : 2.11  
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) : 2.11

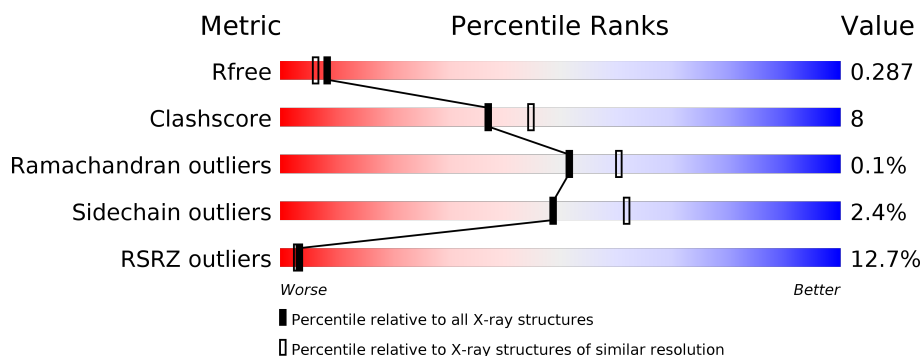
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	208	<div> <div>10%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	B	208	<div> <div>9%</div> <div>84%</div> <div>13%</div> <div>..</div> </div>
1	C	208	<div> <div>17%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
1	D	208	<div> <div>13%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6269 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.

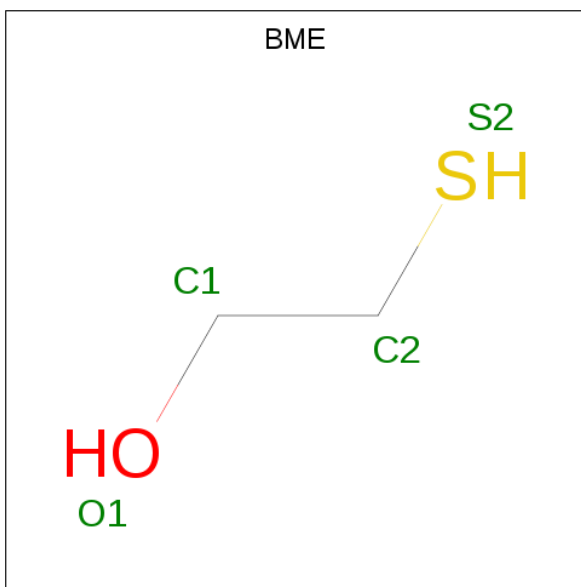
- Molecule 1 is a protein called Carbonic anhydrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1580	1008	276	291	5			
1	B	205	Total	C	N	O	S	0	0	0
			1568	1003	276	284	5			
1	C	204	Total	C	N	O	S	0	0	0
			1518	962	267	284	5			
1	D	202	Total	C	N	O	S	0	0	0
			1532	975	270	282	5			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

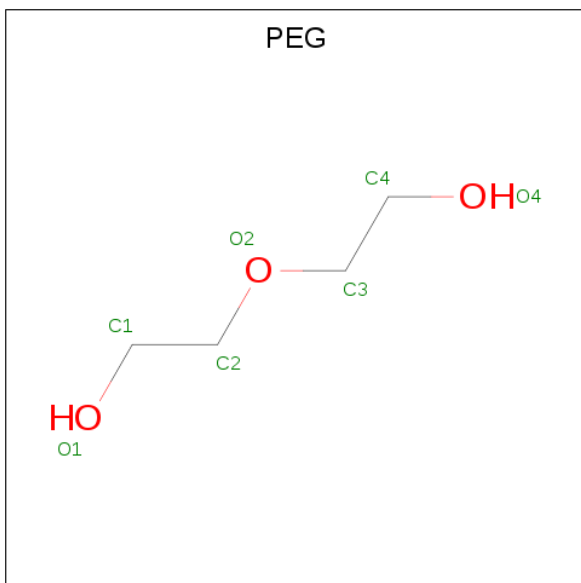
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



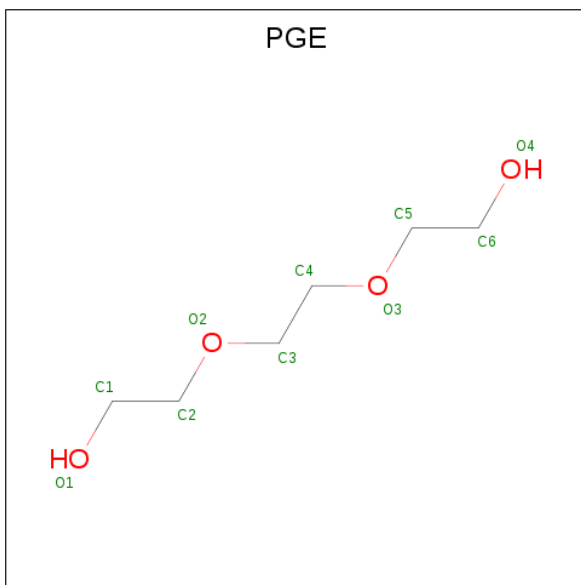
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	S	0	0
			2	1	1		
3	A	1	Total	C	O	S	0
			4	2	1	1	
3	C	1	Total	S		0	0
			1	1			
3	D	1	Total	S		0	0
			1	1			

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	6	4		

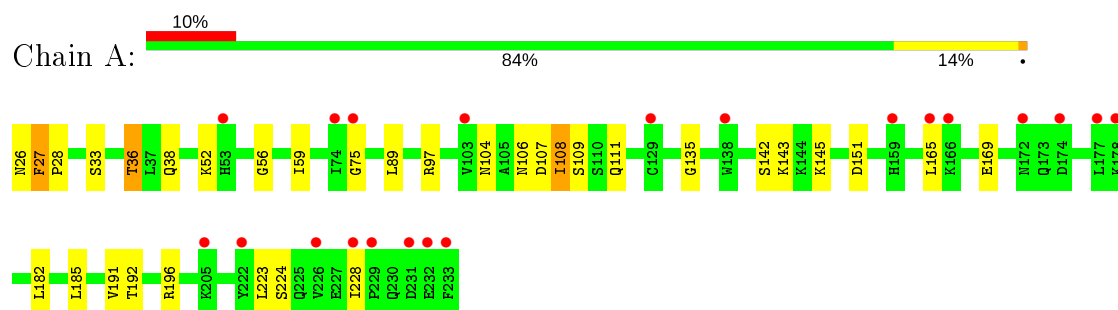
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	11	Total	O	0	0
			11	11		
6	C	5	Total	O	0	0
			5	5		
6	D	5	Total	O	0	0
			5	5		

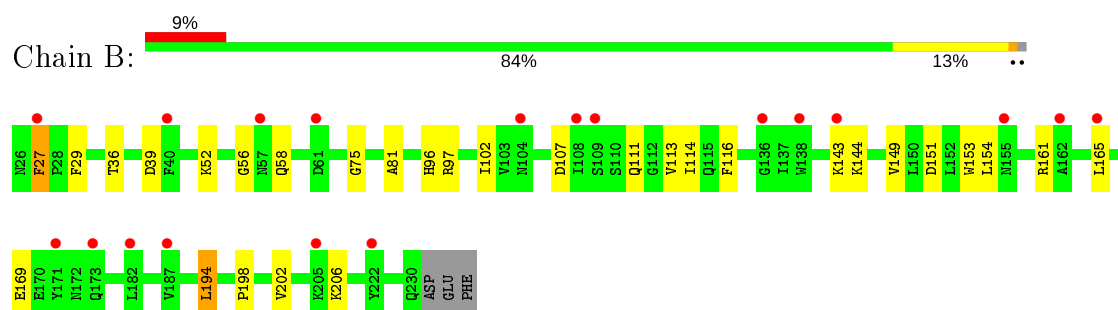
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

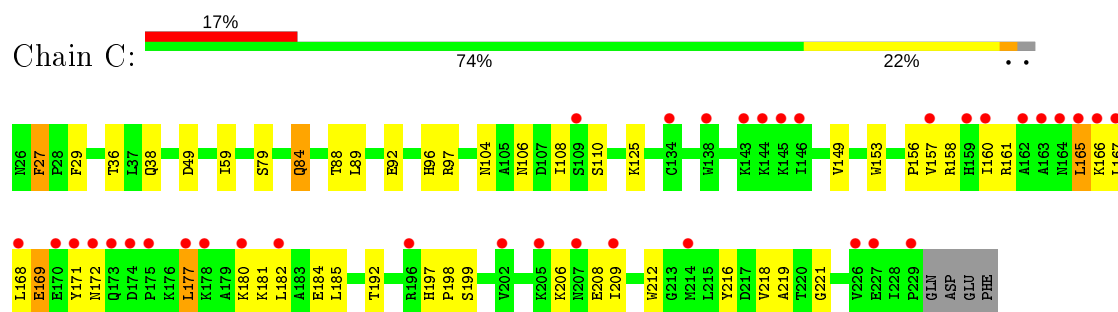
#### • Molecule 1: Carbonic anhydrase



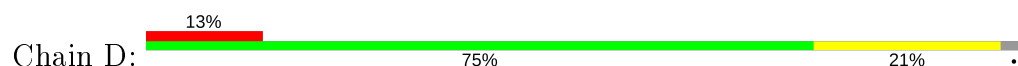
#### • Molecule 1: Carbonic anhydrase

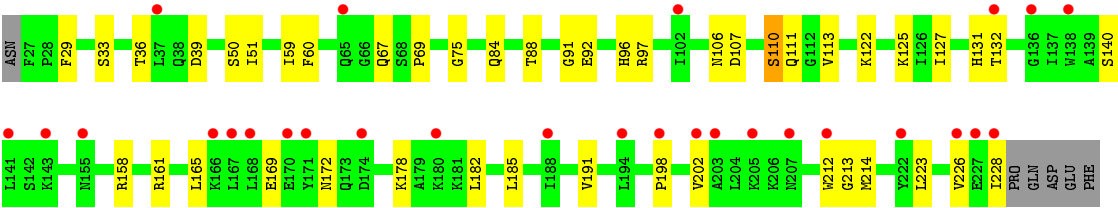


#### • Molecule 1: Carbonic anhydrase



#### • Molecule 1: Carbonic anhydrase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.36 Å 90.28 Å 167.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.94 – 2.20 45.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.94-2.20) 98.5 (45.94-2.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.20 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.241 , 0.279 0.243 , 0.287	Depositor DCC
$R_{free}$ test set	809 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	1.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PEG, PGE, BME

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	0.99	2/1612 (0.1%)	0.81	1/2189 (0.0%)
1	B	0.99	0/1600	0.80	1/2172 (0.0%)
1	C	0.90	3/1546 (0.2%)	0.82	2/2105 (0.1%)
1	D	0.91	0/1561	0.77	1/2120 (0.0%)
All	All	0.95	5/6319 (0.1%)	0.80	5/8586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	SER	CB-OG	6.83	1.51	1.42
1	C	96	HIS	N-CA	-6.45	1.33	1.46
1	A	135	GLY	CA-C	5.41	1.60	1.51
1	C	84	GLN	N-CA	5.25	1.56	1.46
1	C	49	ASP	N-CA	5.08	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	LEU	CA-CB-CG	7.86	133.39	115.30
1	A	223	LEU	CA-CB-CG	6.60	130.48	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	97	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	81	ALA	C-N-CA	-5.48	110.78	122.30
1	D	223	LEU	CA-CB-CG	5.41	127.74	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	27	PHE	Peptide
1	C	169	GLU	Peptide
1	C	27	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	1580	0	1558	19	0
1	B	1568	0	1566	19	0
1	C	1518	0	1470	38	0
1	D	1532	0	1514	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	6	0	5	1	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	20	0	0
5	B	10	0	14	0	0
6	A	14	0	0	0	0
6	B	11	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
All	All	6269	0	6147	97	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 (97) 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:C:180:LYS:O	1:C:184:GLU:HG3	1.80	0.81
1:A:191:VAL:HG11	1:A:228:ILE:HD13	1.67	0.77
1:B:143:LYS:HE2	1:B:161:ARG:HH12	1.50	0.77
1:C:166:LYS:HE2	1:C:169:GLU:CB	2.21	0.70
1:D:51:ILE:CG2	1:D:59:ILE:HG21	2.22	0.70
1:D:169:GLU:O	1:D:172:ASN:HB2	1.91	0.70
1:C:180:LYS:NZ	1:C:184:GLU:OE1	2.25	0.69
1:A:104:ASN:ND2	1:A:106:ASN:OD1	2.29	0.65
1:A:59:ILE:HD11	1:A:89:LEU:HD13	1.80	0.63
1:C:169:GLU:CB	1:C:172:ASN:HB2	2.30	0.61
1:B:107:ASP:O	1:B:111:GLN:HG2	2.01	0.60
1:A:106:ASN:HD21	1:D:106:ASN:HB2	1.67	0.60
1:C:171:TYR:CE1	1:C:177:LEU:HD22	2.37	0.60
1:D:96:HIS:HB2	1:D:113:VAL:HG11	1.84	0.60
1:C:157:VAL:HA	1:C:160:ILE:HD12	1.86	0.58
1:D:51:ILE:HG23	1:D:59:ILE:HG21	1.86	0.57
1:A:107:ASP:O	1:A:111:GLN:HG2	2.05	0.57
1:C:182:LEU:HA	1:C:185:LEU:HD12	1.87	0.57
1:C:165:LEU:HD23	1:C:167:LEU:HB2	1.88	0.56
1:B:96:HIS:HB2	1:B:113:VAL:HG11	1.88	0.55
3:A:303:BME:H12	1:B:116:PHE:CE2	2.42	0.55
1:A:108:ILE:HG13	1:B:149:VAL:CG1	2.37	0.55
1:C:197:HIS:CD2	1:C:199:SER:H	2.26	0.54
1:D:158:ARG:HG2	1:D:161:ARG:HH11	1.72	0.54
1:C:36:THR:HG22	1:C:38:GLN:H	1.73	0.53
1:B:114:ILE:HD13	1:B:194:LEU:HD12	1.91	0.53
1:C:169:GLU:C	1:C:171:TYR:H	2.11	0.53
1:D:107:ASP:OD2	1:D:110:SER:OG	2.25	0.53
1:D:213:GLY:O	1:D:226:VAL:N	2.42	0.52
1:A:52:LYS:HA	1:A:56:GLY:O	2.10	0.52
1:D:36:THR:CG2	1:D:39:ASP:H	2.23	0.52
1:D:67:GLN:HG3	1:D:69:PRO:HD3	1.91	0.51
1:B:36:THR:HG22	1:B:39:ASP:CG	2.31	0.51
1:D:36:THR:HG23	1:D:39:ASP:H	1.76	0.50
1:C:158:ARG:HH21	1:C:158:ARG:HG2	1.76	0.50
1:A:108:ILE:HG13	1:B:149:VAL:HG13	1.94	0.50
1:B:27:PHE:HB3	1:B:29:PHE:H	1.77	0.50
1:A:182:LEU:HA	1:A:185:LEU:HD12	1.94	0.49
1:C:165:LEU:HG	1:C:166:LYS:H	1.77	0.49
1:D:107:ASP:O	1:D:111:GLN:HG2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:HIS:ND1	1:D:132:THR:O	2.43	0.49
1:C:104:ASN:OD1	1:C:106:ASN:HB2	2.13	0.48
1:B:52:LYS:HA	1:B:56:GLY:O	2.14	0.48
1:D:36:THR:HG22	1:D:39:ASP:CG	2.34	0.48
1:C:177:LEU:HD23	1:C:177:LEU:O	2.14	0.48
1:D:172:ASN:HA	1:D:178:LYS:HE3	1.95	0.48
1:C:125:LYS:HD3	1:C:212:TRP:CH2	2.48	0.48
1:C:165:LEU:HG	1:C:167:LEU:N	2.30	0.47
1:C:88:THR:O	1:D:84:GLN:NE2	2.48	0.46
1:A:192:THR:O	1:A:196:ARG:HG3	2.15	0.46
1:C:59:ILE:HD11	1:C:89:LEU:HD13	1.98	0.46
1:B:75:GLY:O	1:B:97:ARG:HA	2.16	0.46
1:A:36:THR:HG22	1:A:38:GLN:N	2.30	0.46
1:C:165:LEU:CG	1:C:166:LYS:H	2.28	0.45
1:C:161:ARG:HG3	1:C:168:LEU:CD2	2.46	0.45
1:C:171:TYR:CD1	1:C:177:LEU:HD22	2.51	0.45
1:C:197:HIS:HD2	1:C:199:SER:H	1.64	0.45
1:C:79:SER:OG	1:D:91:GLY:HA2	2.15	0.45
1:D:191:VAL:HG11	1:D:228:ILE:HD13	1.98	0.45
1:A:142:SER:OG	1:A:143:LYS:N	2.49	0.45
1:A:145:LYS:HE2	1:A:145:LYS:HB3	1.71	0.45
1:C:84:GLN:NE2	1:D:88:THR:O	2.45	0.45
1:D:51:ILE:CG2	1:D:59:ILE:CG2	2.94	0.45
1:D:51:ILE:HG21	1:D:59:ILE:HG21	1.98	0.45
1:A:145:LYS:HG2	1:A:151:ASP:OD2	2.17	0.45
1:C:208:GLU:O	1:C:209:ILE:HG13	2.17	0.45
1:A:165:LEU:O	1:A:169:GLU:HG3	2.17	0.44
1:B:102:ILE:HD12	1:B:153:TRP:NE1	2.33	0.44
1:D:125:LYS:HD3	1:D:212:TRP:CH2	2.53	0.44
1:D:75:GLY:O	1:D:97:ARG:HA	2.18	0.44
1:A:75:GLY:O	1:A:97:ARG:HA	2.18	0.44
1:C:153:TRP:O	1:C:156:PRO:HD2	2.18	0.43
1:D:127:ILE:HG23	1:D:214:MET:HG3	2.00	0.43
1:B:198:PRO:O	1:B:202:VAL:HG13	2.17	0.43
1:A:28:PRO:HG3	1:B:58:GLN:NE2	2.33	0.43
1:D:122:LYS:N	1:D:122:LYS:HD2	2.33	0.43
1:A:26:ASN:HA	1:A:27:PHE:HA	1.71	0.43
1:B:143:LYS:HE2	1:B:161:ARG:NH1	2.27	0.43
1:B:165:LEU:O	1:B:169:GLU:HG3	2.18	0.43
1:C:161:ARG:HG3	1:C:168:LEU:HD22	2.00	0.42
1:C:92:GLU:CD	1:D:29:PHE:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ALA:O	1:D:60:PHE:HB3	2.18	0.42
1:C:27:PHE:HB3	1:C:29:PHE:HD2	1.85	0.42
1:C:216:TYR:CE2	1:C:218:VAL:HA	2.55	0.42
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.87	0.41
1:C:216:TYR:CE1	1:C:221:GLY:HA2	2.55	0.41
1:D:158:ARG:CG	1:D:161:ARG:HH11	2.33	0.41
1:D:182:LEU:HA	1:D:185:LEU:HD12	2.03	0.41
1:D:198:PRO:O	1:D:202:VAL:HG23	2.20	0.41
1:B:151:ASP:HB3	1:C:198:PRO:HG3	2.03	0.41
1:C:158:ARG:HG2	1:C:158:ARG:NH2	2.36	0.41
1:C:165:LEU:HG	1:C:167:LEU:H	1.84	0.41
1:B:202:VAL:O	1:B:206:LYS:HG3	2.21	0.41
1:A:59:ILE:CD1	1:A:89:LEU:HD13	2.48	0.41
1:C:206:LYS:HE3	1:C:208:GLU:OE2	2.19	0.40
1:C:29:PHE:HB3	1:D:92:GLU:CD	2.41	0.40
1:D:140:SER:O	1:D:161:ARG:NE	2.51	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	206/208 (99%)	201 (98%)	4 (2%)	1 (0%)	29	31
1	B	203/208 (98%)	198 (98%)	5 (2%)	0	100	100
1	C	202/208 (97%)	187 (93%)	15 (7%)	0	100	100
1	D	198/208 (95%)	186 (94%)	12 (6%)	0	100	100
All	All	809/832 (97%)	772 (95%)	36 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	PHE

### 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	168/180 (93%)	164 (98%)	4 (2%)	49	62
1	B	168/180 (93%)	166 (99%)	2 (1%)	71	83
1	C	159/180 (88%)	153 (96%)	6 (4%)	33	42
1	D	164/180 (91%)	160 (98%)	4 (2%)	49	62
All	All	659/720 (92%)	643 (98%)	16 (2%)	49	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	36	THR
1	A	108	ILE
1	A	224	SER
1	B	144	LYS
1	B	194	LEU
1	C	108	ILE
1	C	110	SER
1	C	149	VAL
1	C	177	LEU
1	C	181	LYS
1	C	192	THR
1	D	33	SER
1	D	50	SER
1	D	110	SER
1	D	165	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	106	ASN
1	B	159	HIS
1	C	55	HIS
1	C	172	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 5 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	$\# Z  > 2$
4	PEG	A	304	-	6,6,6	0.74	0	5,5,5	0.35	0
5	PGE	B	302	-	9,9,9	0.64	0	8,8,8	0.23	0
3	BME	A	303	2	3,3,3	0.22	0	1,2,2	1.33	0
3	BME	A	302	2	0,1,3	0.00	-	-		
4	PEG	A	305	-	6,6,6	0.62	0	5,5,5	0.47	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
4	PEG	A	304	-	-	2/4/4/4	-
5	PGE	B	302	-	-	5/7/7/7	-
3	BME	A	303	2	-	0/1/1/1	-
4	PEG	A	305	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	302	PGE	O1-C1-C2-O2
5	B	302	PGE	O3-C5-C6-O4
4	A	304	PEG	O1-C1-C2-O2
4	A	304	PEG	O2-C3-C4-O4
5	B	302	PGE	C1-C2-O2-C3
5	B	302	PGE	C6-C5-O3-C4
5	B	302	PGE	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	303	BME	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	225:GLN	C	226:VAL	N	2.75

## 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	208/208 (100%)	0.93	21 (10%) 7 6	51, 72, 118, 150	0
1	B	205/208 (98%)	0.85	19 (9%) 8 7	53, 72, 112, 138	1 (0%)
1	C	204/208 (98%)	1.22	36 (17%) 1 1	59, 86, 154, 188	0
1	D	202/208 (97%)	1.03	28 (13%) 2 2	56, 80, 122, 145	0
All	All	819/832 (98%)	1.01	104 (12%) 3 3	51, 78, 125, 188	1 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	PHE	7.4
1	A	231	ASP	6.3
1	D	138	TRP	6.1
1	A	165	LEU	5.8
1	D	207	ASN	5.6
1	C	146	ILE	5.2
1	B	27	PHE	5.2
1	C	173	GLN	5.2
1	C	207	ASN	5.1
1	C	227	GLU	4.8
1	D	226	VAL	4.7
1	C	174	ASP	4.5
1	B	143	LYS	4.4
1	C	171	TYR	4.2
1	D	167	LEU	4.2
1	A	138	TRP	4.0
1	C	196	ARG	3.9
1	C	165	LEU	3.9
1	A	172	ASN	3.8
1	B	173	GLN	3.8
1	C	162	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	37	LEU	3.7
1	D	166	LYS	3.7
1	A	174	ASP	3.7
1	C	172	ASN	3.6
1	C	177	LEU	3.6
1	C	178	LYS	3.5
1	D	203	ALA	3.5
1	C	167	LEU	3.4
1	A	166	LYS	3.4
1	C	168	LEU	3.3
1	C	175	PRO	3.3
1	B	222	TYR	3.2
1	D	227	GLU	3.2
1	C	226	VAL	3.2
1	A	229	PRO	3.1
1	D	212	TRP	3.0
1	D	222	TYR	3.0
1	B	182	LEU	3.0
1	C	209	ILE	2.9
1	D	180	LYS	2.9
1	A	232	GLU	2.9
1	D	136	GLY	2.8
1	D	65	GLN	2.8
1	D	155	ASN	2.8
1	A	226	VAL	2.7
1	D	143	LYS	2.7
1	C	160	ILE	2.7
1	A	205	LYS	2.7
1	B	108	ILE	2.7
1	D	205	LYS	2.7
1	C	145	LYS	2.6
1	C	205	LYS	2.6
1	C	164	ASN	2.6
1	C	109	SER	2.6
1	D	228	ILE	2.6
1	C	202	VAL	2.6
1	A	74	ILE	2.6
1	D	198	PRO	2.6
1	D	174	ASP	2.6
1	A	228	ILE	2.6
1	C	134	CYS	2.5
1	D	171	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	166	LYS	2.5
1	B	187	VAL	2.5
1	A	222	TYR	2.5
1	B	171	TYR	2.5
1	B	155	ASN	2.5
1	A	159	HIS	2.4
1	A	178	LYS	2.4
1	C	157	VAL	2.4
1	D	202	VAL	2.4
1	A	177	LEU	2.3
1	D	194	LEU	2.3
1	C	170	GLU	2.3
1	B	162	ALA	2.3
1	C	163	ALA	2.3
1	D	141	LEU	2.3
1	D	170	GLU	2.3
1	B	165	LEU	2.2
1	C	144	LYS	2.2
1	C	182	LEU	2.2
1	B	57	ASN	2.2
1	A	129	CYS	2.2
1	A	103	VAL	2.2
1	C	138	TRP	2.2
1	C	214	MET	2.2
1	D	168	LEU	2.2
1	B	205	LYS	2.2
1	C	159	HIS	2.2
1	B	138	TRP	2.2
1	A	53	HIS	2.2
1	B	61	ASP	2.2
1	D	102	ILE	2.1
1	B	109	SER	2.1
1	D	188	ILE	2.1
1	C	229	PRO	2.1
1	C	143	LYS	2.1
1	C	180	LYS	2.1
1	B	136	GLY	2.0
1	B	40	PHE	2.0
1	A	75	GLY	2.0
1	D	132	THR	2.0
1	B	104	ASN	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 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. 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
5	PGE	B	302	10/10	0.67	0.19	78,102,108,108	0
4	PEG	A	304	7/7	0.79	0.17	71,81,95,98	0
4	PEG	A	305	7/7	0.81	0.15	70,87,92,94	0
3	BME	A	303	4/4	0.89	0.22	57,65,65,69	0
3	BME	C	302	1/4	0.89	0.27	96,96,96,96	0
3	BME	A	302	2/4	0.92	0.29	69,69,69,88	0
2	ZN	D	301	1/1	0.93	0.15	66,66,66,66	0
2	ZN	B	301	1/1	0.95	0.13	66,66,66,66	0
2	ZN	C	301	1/1	0.95	0.15	79,79,79,79	0
3	BME	D	302	1/4	0.95	0.33	87,87,87,87	0
2	ZN	A	301	1/1	0.97	0.09	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.