



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 PM UTC

PDB ID : 6GWU / pdb_00006gwu
Title : Carbonic anhydrase CaNce103p from Candida albicans
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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

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>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

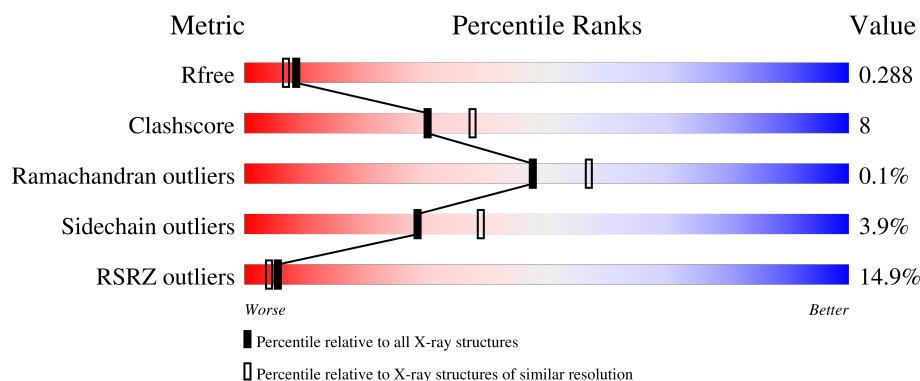
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	11% 76% 21% .
1	B	208	10% 79% 18% ..
1	C	208	25% 69% 25% ..
1	D	208	13% 69% 27% ..

2 Entry composition

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



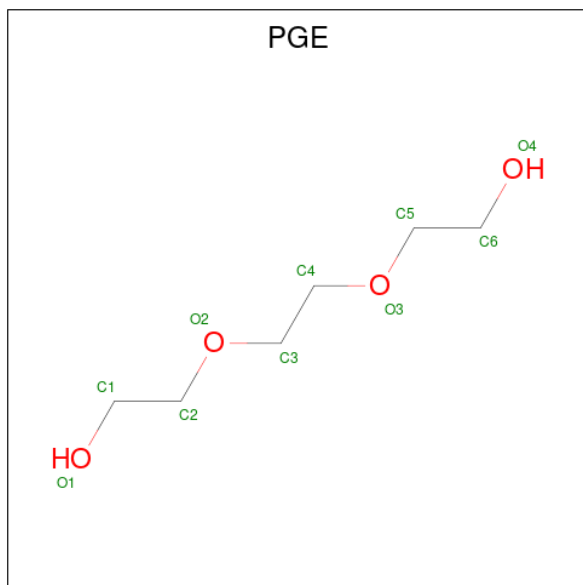
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	S			
			2	1	1	0	0	
3	A	1	Total	C	O	S		
			4	2	1	1	0	
3	C	1	Total	S				
			1	1			0	
3	D	1	Total	S				
			1	1			0	

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: 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 (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

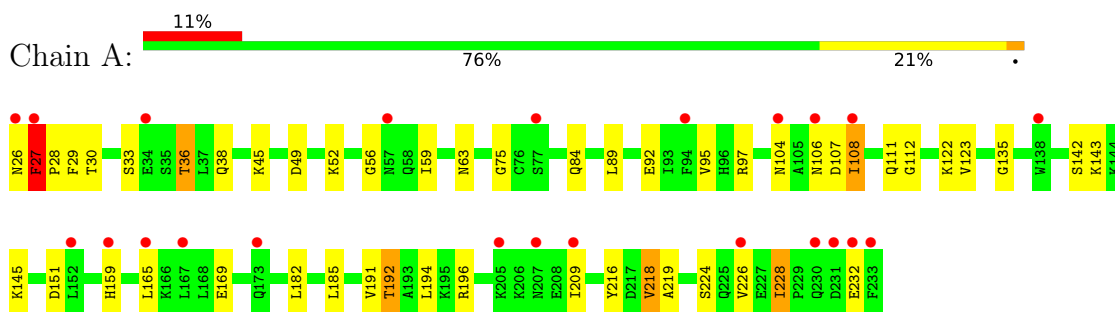
- Molecule 6 is water.

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		

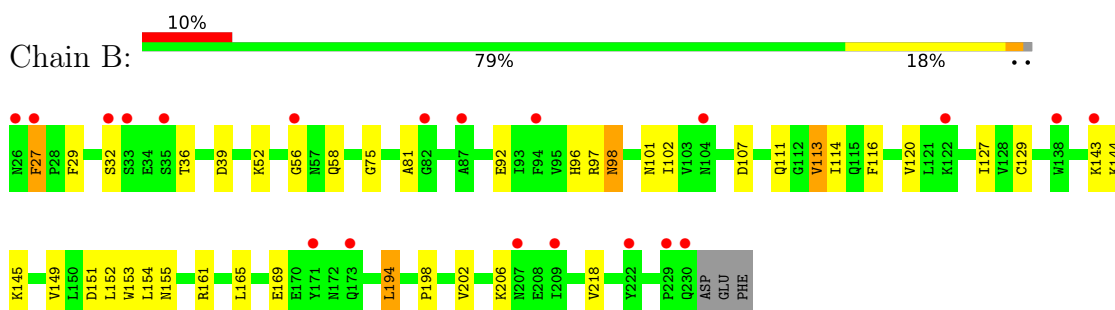
3 Residue-property plots

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.

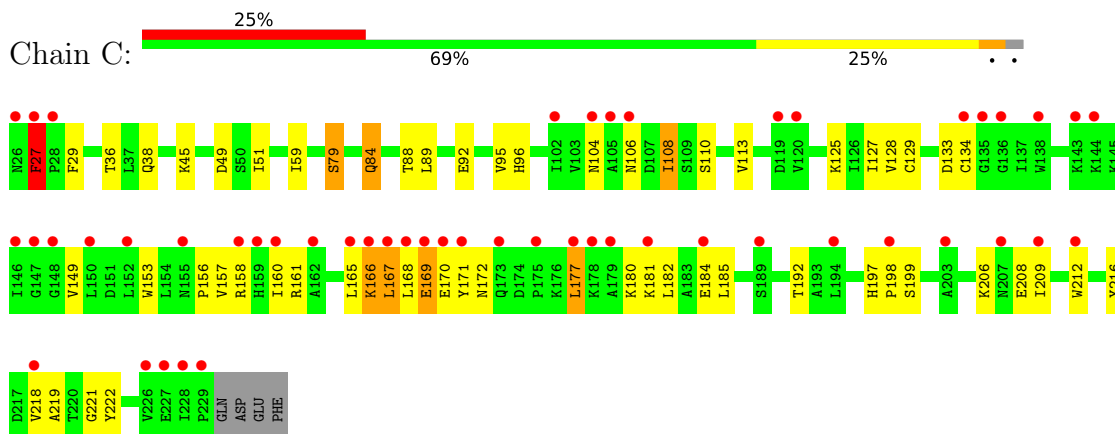
• Molecule 1: Carbonic anhydrase



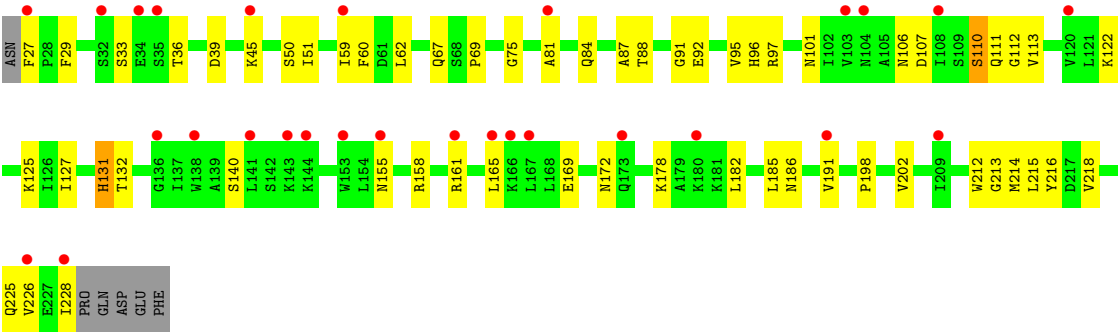
• Molecule 1: Carbonic anhydrase



• 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, α , β , γ	69.36Å 90.28Å 167.10Å 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
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.241 , 0.279 0.243 , 0.288	Depositor DCC
R_{free} test set	809 reflections (1.52%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	1.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: PGE, BME, ZN, PEG

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	1.39	12/1612 (0.7%)	1.15	4/2189 (0.2%)
1	B	1.38	8/1600 (0.5%)	1.12	4/2172 (0.2%)
1	C	1.31	13/1546 (0.8%)	1.15	7/2105 (0.3%)
1	D	1.31	7/1561 (0.4%)	1.16	7/2120 (0.3%)
All	All	1.35	40/6319 (0.6%)	1.15	22/8586 (0.3%)

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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	96	HIS	N-CA	-10.02	1.33	1.46
1	C	49	ASP	N-CA	8.51	1.56	1.46
1	C	84	GLN	N-CA	8.26	1.56	1.46
1	A	216	TYR	N-CA	-7.42	1.37	1.46
1	A	45	LYS	N-CA	7.12	1.55	1.46
1	C	134	CYS	N-CA	7.05	1.55	1.46
1	A	135	GLY	CA-C	7.00	1.60	1.52
1	C	27	PHE	CA-C	6.62	1.58	1.52
1	A	84	GLN	N-CA	6.62	1.54	1.46
1	B	32	SER	CA-C	6.45	1.60	1.52
1	C	127	ILE	CA-CB	6.38	1.62	1.54
1	D	45	LYS	N-CA	6.31	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	ILE	CA-C	-6.20	1.44	1.52
1	A	228	ILE	C-N	5.97	1.41	1.33
1	D	216	TYR	N-CA	-5.95	1.38	1.46
1	B	98	ASN	N-CA	5.91	1.53	1.45
1	A	218	VAL	CA-C	5.82	1.60	1.52
1	A	219	ALA	C-O	-5.69	1.16	1.24
1	B	81	ALA	CA-C	-5.64	1.46	1.53
1	C	129	CYS	N-CA	-5.61	1.39	1.46
1	B	113	VAL	N-CA	5.60	1.53	1.46
1	D	62	LEU	C-O	-5.58	1.17	1.24
1	A	123	VAL	C-O	-5.46	1.17	1.24
1	C	45	LYS	N-CA	5.43	1.52	1.46
1	B	129	CYS	N-CA	-5.40	1.40	1.46
1	C	113	VAL	N-CA	5.38	1.52	1.46
1	B	120	VAL	CA-C	5.28	1.59	1.52
1	A	63	ASN	N-CA	-5.27	1.39	1.46
1	D	215	LEU	CA-C	5.25	1.58	1.52
1	C	108	ILE	CA-CB	5.22	1.63	1.54
1	C	222	TYR	CA-C	5.19	1.59	1.52
1	A	112	GLY	CA-C	5.11	1.57	1.52
1	D	112	GLY	CA-C	5.11	1.57	1.52
1	C	128	VAL	CA-CB	5.10	1.60	1.54
1	A	49	ASP	N-CA	5.07	1.52	1.46
1	B	152	LEU	CA-C	-5.07	1.46	1.52
1	D	87	ALA	C-O	5.07	1.29	1.23
1	D	131	HIS	C-O	-5.06	1.17	1.23
1	C	79	SER	CA-C	5.02	1.59	1.52
1	A	27	PHE	C-N	5.00	1.40	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLU	N-CA-C	-7.46	104.63	113.21
1	C	95	VAL	N-CA-C	6.29	117.54	108.48
1	D	155	ASN	CA-C-N	-6.22	113.22	119.56
1	D	155	ASN	C-N-CA	-6.22	113.22	119.56
1	B	155	ASN	CA-C-N	-6.17	113.27	119.56
1	B	155	ASN	C-N-CA	-6.17	113.27	119.56
1	A	226	VAL	N-CA-CB	6.06	117.33	110.72
1	A	232	GLU	N-CA-C	6.04	121.46	112.94
1	C	129	CYS	N-CA-C	5.86	118.27	108.02
1	D	27	PHE	CA-C-N	5.80	126.75	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	PHE	C-N-CA	5.80	126.75	120.83
1	A	30	THR	N-CA-C	5.79	117.59	111.28
1	C	166	LYS	N-CA-C	-5.75	104.94	112.41
1	A	95	VAL	N-CA-C	5.58	115.92	108.11
1	C	167	LEU	N-CA-C	-5.48	105.31	111.28
1	B	81	ALA	CA-C-N	-5.42	110.78	121.41
1	B	81	ALA	C-N-CA	-5.42	110.78	121.41
1	D	186	ASN	N-CA-C	5.39	117.16	111.28
1	D	95	VAL	N-CA-C	5.31	115.55	108.11
1	D	81	ALA	N-CA-C	-5.28	101.68	109.86
1	C	133	ASP	CA-C-N	5.07	128.53	121.02
1	C	133	ASP	C-N-CA	5.07	128.53	121.02

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 [i](#)

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	21	0
1	B	1568	0	1566	23	0
1	C	1518	0	1470	39	0
1	D	1532	0	1514	34	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	104	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 (104) 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:C:169:GLU:C	1:C:171:TYR:H	2.11	0.57
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:36:THR:HG22	1:B:39:ASP:CG	2.31	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:THR:HG22	1:D:39:ASP:CG	2.34	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:D:36:THR:HG23	1:D:39:ASP:H	1.76	0.50
1:C:158:ARG:HG2	1:C:158:ARG:HH21	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
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: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:92:GLU:CD	1:D:29:PHE:HB3	2.39	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:161:ARG:HG3	1:C:168:LEU:CD2	2.46	0.45
1:C:165:LEU:CG	1:C:166:LYS:H	2.28	0.45
1:C:171:TYR:CD1	1:C:177:LEU:HD22	2.51	0.45
1:C:79:SER:OG	1:D:91:GLY:HA2	2.15	0.45
1:C:197:HIS:HD2	1:C:199:SER:H	1.64	0.45
1:D:191:VAL:HG11	1:D:228:ILE:HD13	1.98	0.45
1:A:145:LYS:HB3	1:A:145:LYS:HE2	1.71	0.45
1:C:29:PHE:HB3	1:D:92:GLU:CD	2.41	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:142:SER:OG	1:A:143:LYS:N	2.49	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:D:225:GLN:C	1:D:226:VAL:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:O	1:A:169:GLU:HG3	2.17	0.44
1:A:92:GLU:CD	1:B:29:PHE:HB3	2.43	0.44
1:B:102:ILE:HD12	1:B:153:TRP:NE1	2.33	0.44
1:D:75:GLY:O	1:D:97:ARG:HA	2.18	0.44
1:D:125:LYS:HD3	1:D:212:TRP:CH2	2.53	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:A:28:PRO:HG3	1:B:58:GLN:NE2	2.33	0.43
1:B:198:PRO:O	1:B:202:VAL:HG13	2.17	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:219:ALA:O	1:D:60:PHE:HB3	2.18	0.42
1:B:75:GLY:C	1:B:101:ASN:HB3	2.45	0.42
1:C:27:PHE:HB3	1:C:29:PHE:HD2	1.85	0.42
1:C:169:GLU:C	1:C:171:TYR:N	2.78	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:29:PHE:HB3	1:B:92:GLU:CD	2.46	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:B:98:ASN:OD1	1:B:98:ASN:C	2.64	0.40
1:D:75:GLY:C	1:D:101:ASN:HB3	2.47	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%)	24	27
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%)	48	57

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%)	158 (94%)	10 (6%)	17	21
1	B	168/180 (93%)	164 (98%)	4 (2%)	43	58
1	C	159/180 (88%)	152 (96%)	7 (4%)	25	34
1	D	164/180 (91%)	159 (97%)	5 (3%)	36	49
All	All	659/720 (92%)	633 (96%)	26 (4%)	28	39

All (26) 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	122	LYS
1	A	159	HIS
1	A	192	THR
1	A	194	LEU
1	A	209	ILE
1	A	218	VAL
1	A	224	SER
1	B	144	LYS
1	B	145	LYS
1	B	194	LEU
1	B	218	VAL
1	C	51	ILE
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
1	D	218	VAL

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	43	ASN
1	A	57	ASN
1	A	104	ASN
1	A	106	ASN
1	B	53	HIS
1	B	55	HIS
1	B	58	GLN
1	B	84	GLN
1	B	159	HIS
1	B	225	GLN
1	C	53	HIS
1	C	55	HIS
1	C	172	ASN

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Mol	Chain	Res	Type
1	D	55	HIS
1	D	186	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 oligosaccharides 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	$\# Z > 2$
3	BME	A	302	2	0,1,3	-	-	-		
4	PEG	A	304	-	6,6,6	0.75	0	5,5,5	0.35	0
3	BME	A	303	2	3,3,3	0.15	0	2,2,2	1.38	0
4	PEG	A	305	-	6,6,6	0.62	0	5,5,5	0.47	0
5	PGE	B	302	-	9,9,9	0.65	0	8,8,8	0.22	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	-
4	PEG	A	305	-	-	0/4/4/4	-
3	BME	A	303	2	-	0/1/1/1	-
5	PGE	B	302	-	-	5/7/7/7	-

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
4	A	304	PEG	O1-C1-C2-O2
4	A	304	PEG	O2-C3-C4-O4
5	B	302	PGE	O3-C5-C6-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, 95th 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 ²)	Q<0.9
1	A	208/208 (100%)	1.12	23 (11%) 10 8	51, 72, 118, 150	0
1	B	205/208 (98%)	1.09	20 (9%) 13 10	53, 72, 112, 138	1 (0%)
1	C	204/208 (98%)	1.54	51 (25%) 2 1	59, 86, 154, 188	0
1	D	202/208 (97%)	1.29	28 (13%) 6 5	56, 80, 122, 145	0
All	All	819/832 (98%)	1.26	122 (14%) 5 4	51, 77, 125, 188	1 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	LEU	6.4
1	C	168	LEU	6.4
1	D	27	PHE	5.9
1	B	26	ASN	5.8
1	B	27	PHE	5.7
1	A	233	PHE	5.5
1	B	138	TRP	5.3
1	D	165	LEU	4.9
1	C	26	ASN	4.9
1	A	27	PHE	4.7
1	C	27	PHE	4.7
1	D	59	ILE	4.2
1	C	167	LEU	4.0
1	A	26	ASN	4.0
1	A	232	GLU	3.8
1	C	189	SER	3.7
1	C	159	HIS	3.6
1	B	230	GLN	3.6
1	C	209	ILE	3.6
1	C	143	LYS	3.5
1	B	207	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	146	ILE	3.5
1	A	231	ASP	3.5
1	A	226	VAL	3.4
1	A	173	GLN	3.4
1	C	166	LYS	3.3
1	D	143	LYS	3.3
1	A	108	ILE	3.2
1	C	162	ALA	3.2
1	C	227	GLU	3.2
1	D	155	ASN	3.2
1	C	171	TYR	3.1
1	A	57	ASN	3.1
1	A	230	GLN	3.1
1	C	198	PRO	3.1
1	C	184	GLU	3.1
1	D	138	TRP	3.1
1	A	94	PHE	3.1
1	D	226	VAL	3.0
1	C	228	ILE	3.0
1	A	207	ASN	3.0
1	B	209	ILE	3.0
1	C	160	ILE	3.0
1	C	177	LEU	2.9
1	C	207	ASN	2.9
1	C	144	LYS	2.9
1	A	138	TRP	2.8
1	D	144	LYS	2.8
1	C	147	GLY	2.8
1	C	28	PRO	2.8
1	D	166	LYS	2.8
1	B	32	SER	2.8
1	D	136	GLY	2.8
1	C	173	GLN	2.7
1	C	179	ALA	2.7
1	C	226	VAL	2.7
1	C	136	GLY	2.7
1	C	150	LEU	2.7
1	B	33	SER	2.7
1	C	152	LEU	2.7
1	D	167	LEU	2.7
1	D	161	ARG	2.6
1	D	228	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	103	VAL	2.6
1	A	165	LEU	2.6
1	A	104	ASN	2.6
1	A	167	LEU	2.5
1	D	141	LEU	2.5
1	D	173	GLN	2.5
1	C	194	LEU	2.5
1	C	148	GLY	2.5
1	D	81	ALA	2.5
1	C	102	ILE	2.4
1	B	143	LYS	2.4
1	C	119	ASP	2.4
1	C	105	ALA	2.4
1	C	169	GLU	2.4
1	D	45	LYS	2.4
1	B	222	TYR	2.4
1	C	158	ARG	2.4
1	D	34	GLU	2.4
1	C	229	PRO	2.4
1	B	35	SER	2.4
1	D	108	ILE	2.4
1	C	134	CYS	2.4
1	C	218	VAL	2.4
1	C	104	ASN	2.3
1	B	229	PRO	2.3
1	C	175	PRO	2.3
1	B	171	TYR	2.3
1	C	135	GLY	2.3
1	D	209	ILE	2.3
1	D	153	TRP	2.3
1	A	106	ASN	2.2
1	B	82	GLY	2.2
1	C	212	TRP	2.2
1	A	159	HIS	2.2
1	A	77	SER	2.2
1	A	152	LEU	2.2
1	D	104	ASN	2.2
1	C	155	ASN	2.2
1	B	173	GLN	2.2
1	C	106	ASN	2.1
1	C	178	LYS	2.1
1	C	203	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	209	ILE	2.1
1	D	180	LYS	2.1
1	C	170	GLU	2.1
1	D	191	VAL	2.1
1	B	94	PHE	2.1
1	D	32	SER	2.1
1	B	87	ALA	2.1
1	B	122	LYS	2.1
1	C	181	LYS	2.1
1	D	120	VAL	2.1
1	B	56	GLY	2.1
1	A	34	GLU	2.0
1	B	104	ASN	2.0
1	C	120	VAL	2.0
1	A	205	LYS	2.0
1	C	138	TRP	2.0
1	D	35	SER	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 oligosaccharides 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, 95th 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(Å ²)	Q<0.9
5	PGE	B	302	10/10	0.73	0.23	78,102,108,108	0
4	PEG	A	305	7/7	0.82	0.19	70,87,92,94	0
4	PEG	A	304	7/7	0.85	0.19	71,81,95,98	0
3	BME	C	302	1/4	0.88	0.27	96,96,96,96	0
3	BME	A	302	2/4	0.89	0.23	69,69,69,88	0
3	BME	D	302	1/4	0.93	0.25	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BME	A	303	4/4	0.93	0.17	57,65,65,69	0
2	ZN	C	301	1/1	0.98	0.07	79,79,79,79	0
2	ZN	D	301	1/1	0.98	0.05	66,66,66,66	0
2	ZN	B	301	1/1	0.98	0.06	66,66,66,66	0
2	ZN	A	301	1/1	0.99	0.05	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.