



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:18 PM UTC

PDB ID : 1T75 / pdb_00001t75
Title : Crystal structure of Escherichia coli beta carbonic anhydrase
Authors : Oganessian, V.; Kim, S.-H.; Kim, R.; Jancarik, J.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-05-07
Resolution : 2.50 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
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

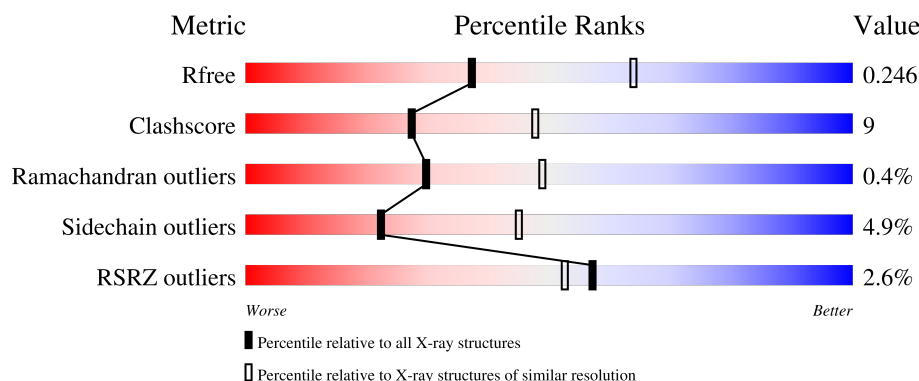
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	220	2% 73% 19% 5%
1	B	220	5% 79% 14%
1	D	220	% 80% 15%
1	E	220	2% 78% 18%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7058 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 Protein yadF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1715	1087	306	313	9			
1	B	214	Total	C	N	O	S	0	0	0
			1715	1087	306	313	9			
1	D	214	Total	C	N	O	S	0	0	0
			1715	1087	306	313	9			
1	E	214	Total	C	N	O	S	0	0	0
			1715	1087	306	313	9			

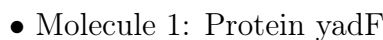
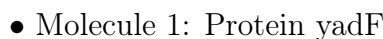
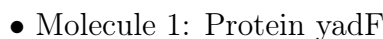
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

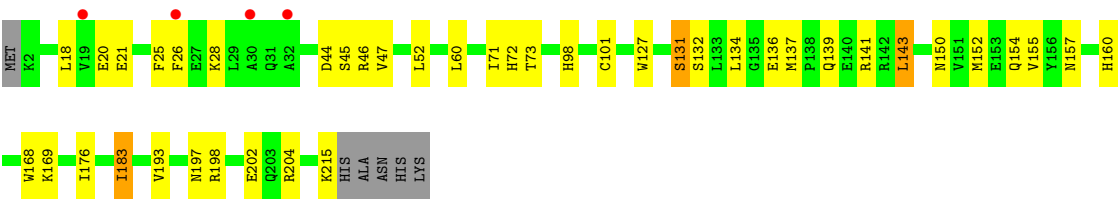
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	66	Total	O	0	0
			66	66		
3	D	43	Total	O	0	0
			43	43		
3	E	51	Total	O	0	0
			51	51		

- Molecule 1: Protein yadF





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	110.45Å 110.45Å 162.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.50 91.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (91.29-2.50) 97.8 (91.29-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.196 , 0.246 0.204 , 0.246	Depositor DCC
R_{free} test set	1750 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 23.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7058	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: ZN

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	0.97	6/1752 (0.3%)	1.43	26/2376 (1.1%)
1	B	1.11	3/1752 (0.2%)	1.24	15/2376 (0.6%)
1	D	0.88	1/1752 (0.1%)	1.02	3/2376 (0.1%)
1	E	0.94	1/1752 (0.1%)	0.99	1/2376 (0.0%)
All	All	0.98	11/7008 (0.2%)	1.18	45/9504 (0.5%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	15	SER	C-N	-23.92	1.02	1.33
1	A	26	PHE	C-N	-9.39	1.20	1.33
1	A	19	VAL	CA-C	-7.88	1.41	1.52
1	B	22	ASP	C-N	-7.49	1.26	1.34
1	D	152	MET	SD-CE	-7.43	1.60	1.79
1	A	152	MET	SD-CE	-7.14	1.61	1.79
1	E	152	MET	SD-CE	-6.47	1.63	1.79
1	A	27	GLU	CB-CG	-6.10	1.34	1.52
1	B	31	GLN	N-CA	-5.32	1.39	1.46
1	A	22	ASP	N-CA	5.29	1.53	1.46
1	A	19	VAL	C-N	-5.14	1.26	1.33

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	PRO	CA-N-CD	-20.53	83.26	112.00
1	B	23	PRO	CA-N-CD	-15.71	90.01	112.00
1	A	48	PRO	CA-N-CD	-15.07	90.91	112.00
1	B	15	SER	CA-C-N	-11.43	104.72	120.38
1	B	15	SER	C-N-CA	-11.43	104.72	120.38
1	A	23	PRO	CA-N-CD	-10.71	97.00	112.00
1	A	27	GLU	CA-CB-CG	10.56	135.23	114.10
1	B	33	GLN	OE1-CD-NE2	-9.98	112.62	122.60
1	A	31	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	203	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	33	GLN	OE1-CD-NE2	-9.77	112.83	122.60
1	B	31	GLN	OE1-CD-NE2	-9.09	113.51	122.60
1	A	27	GLU	CB-CG-CD	8.11	126.39	112.60
1	A	19	VAL	CB-CA-C	-7.76	99.69	112.26
1	B	31	GLN	CB-CA-C	7.21	125.06	109.99
1	B	31	GLN	CG-CD-NE2	7.06	126.99	116.40
1	A	70	VAL	CB-CA-C	6.84	118.14	111.23
1	A	203	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	33	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	20	GLU	CB-CA-C	6.65	119.80	109.03
1	A	19	VAL	CA-C-N	-6.59	111.03	122.36
1	A	19	VAL	C-N-CA	-6.59	111.03	122.36
1	A	26	PHE	CA-C-N	-6.54	109.39	120.58
1	A	26	PHE	C-N-CA	-6.54	109.39	120.58
1	A	31	GLN	CG-CD-NE2	6.46	126.08	116.40
1	B	33	GLN	CG-CD-NE2	6.38	125.97	116.40
1	B	30	ALA	CA-C-N	-6.21	110.28	121.14
1	B	30	ALA	C-N-CA	-6.21	110.28	121.14
1	A	20	GLU	CA-CB-CG	6.13	126.37	114.10
1	B	31	GLN	N-CA-C	-6.12	105.30	112.89
1	D	60	LEU	N-CA-C	6.12	119.47	109.06
1	A	35	PRO	N-CA-CB	6.12	109.14	103.39
1	E	131	SER	N-CA-C	6.09	118.69	111.33
1	B	23	PRO	N-CA-C	6.05	122.44	114.27
1	A	35	PRO	CB-CA-C	-5.84	103.59	111.12
1	D	186	GLY	N-CA-C	-5.84	106.44	116.01
1	D	184	HIS	N-CA-C	-5.73	106.16	114.12
1	A	31	GLN	N-CA-C	-5.63	105.51	112.38
1	A	206	ARG	CA-C-N	5.37	127.73	120.38
1	A	206	ARG	C-N-CA	5.37	127.73	120.38
1	A	61	PHE	N-CA-C	-5.35	100.98	109.76
1	B	25	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	4	ILE	N-CA-C	5.31	120.39	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	ASP	C-N-CD	-5.20	103.70	125.00
1	A	22	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	15	SER	Mainchain

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	1715	0	1699	46	0
1	B	1715	0	1698	50	1
1	D	1715	0	1699	23	0
1	E	1715	0	1699	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	34	0	0	0	0
3	B	66	0	0	6	0
3	D	43	0	0	2	0
3	E	51	0	0	0	0
All	All	7058	0	6795	124	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:23:PRO:HG3	1.32	1.26
1:D:185:ASP:O	1:E:26:PHE:CZ	1.89	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:23:PRO:CG	1.88	1.22
1:B:13:LEU:O	1:B:17:MET:HG3	1.49	1.07
1:B:19:VAL:O	1:B:23:PRO:CD	2.03	1.06
1:A:66:VAL:HG23	3:B:260:HOH:O	1.63	0.98
1:B:13:LEU:O	1:B:17:MET:CG	2.17	0.92
1:B:2:LYS:NZ	3:B:278:HOH:O	2.04	0.91
1:A:39:TRP:HB2	1:A:60:LEU:HD11	1.52	0.90
1:A:156:TYR:OH	1:A:202:GLU:OE2	1.88	0.90
1:D:185:ASP:O	1:E:26:PHE:CE1	2.28	0.86
1:B:141:ARG:HD3	3:B:248:HOH:O	1.77	0.84
1:A:25:PHE:CD2	1:A:26:PHE:CD2	2.68	0.81
1:A:22:ASP:O	1:A:24:GLY:N	2.14	0.80
1:B:3:ASP:OD1	1:B:4:ILE:N	2.14	0.80
1:D:185:ASP:O	1:E:26:PHE:HZ	1.59	0.80
1:D:185:ASP:N	1:D:185:ASP:OD1	2.16	0.79
1:A:66:VAL:O	1:A:67:ALA:HB3	1.83	0.78
1:A:25:PHE:HD2	1:A:26:PHE:CD2	2.03	0.76
1:A:152:MET:HG2	1:A:193:VAL:HG11	1.67	0.76
1:A:17:MET:O	1:A:21:GLU:HB2	1.87	0.75
1:A:25:PHE:CE2	1:A:26:PHE:CE2	2.74	0.75
1:A:37:PHE:HE2	1:B:4:ILE:HD13	1.50	0.75
1:B:141:ARG:CD	3:B:248:HOH:O	2.34	0.75
1:A:166:SER:O	1:A:170:ARG:HG2	1.88	0.72
1:D:185:ASP:C	1:E:26:PHE:CZ	2.67	0.72
1:A:22:ASP:C	1:A:24:GLY:H	2.00	0.69
1:A:11:ASN:HD21	1:B:188:LEU:H	1.43	0.66
1:A:37:PHE:HE2	1:B:4:ILE:CD1	2.09	0.65
1:D:29:LEU:HD21	1:D:57:PRO:HB2	1.79	0.65
1:A:25:PHE:CD2	1:A:26:PHE:CE2	2.86	0.63
1:A:37:PHE:CZ	1:B:2:LYS:O	2.54	0.60
1:A:37:PHE:HZ	1:B:2:LYS:O	1.84	0.59
1:D:177:HIS:ND1	3:D:257:HOH:O	2.32	0.59
1:A:29:LEU:HB3	1:B:183:ILE:HG23	1.85	0.59
1:A:66:VAL:O	1:A:67:ALA:CB	2.51	0.58
1:B:150:ASN:O	1:B:154:GLN:HG2	2.02	0.58
1:B:22:ASP:N	1:B:23:PRO:HD2	2.19	0.58
1:B:19:VAL:HG22	1:B:26:PHE:CE1	2.38	0.58
1:A:22:ASP:C	1:A:24:GLY:N	2.60	0.57
1:B:19:VAL:C	1:B:23:PRO:CD	2.78	0.57
1:B:19:VAL:CG2	1:B:26:PHE:CE1	2.88	0.57
1:B:13:LEU:O	1:B:17:MET:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:O	1:B:23:PRO:HD3	1.99	0.56
1:A:37:PHE:CE2	1:B:4:ILE:HD13	2.37	0.56
1:D:94:ILE:HD13	1:D:179:TRP:CZ3	2.41	0.56
1:B:19:VAL:HA	1:B:23:PRO:HD3	1.87	0.55
1:A:141:ARG:NH1	1:A:215:LYS:NZ	2.55	0.55
1:B:19:VAL:CG2	1:B:26:PHE:HE1	2.20	0.55
1:E:137:MET:HE3	1:E:141:ARG:HB3	1.89	0.54
1:A:141:ARG:NH1	1:A:215:LYS:HZ1	2.06	0.54
1:B:19:VAL:CA	1:B:23:PRO:HD3	2.38	0.54
1:D:193:VAL:HA	1:D:204:ARG:HB3	1.90	0.54
1:B:19:VAL:C	1:B:23:PRO:HD3	2.33	0.53
1:E:160:HIS:NE2	1:E:202:GLU:OE2	2.41	0.53
1:D:192:ASP:CG	1:D:192:ASP:O	2.50	0.53
1:D:133:LEU:C	1:D:133:LEU:HD23	2.35	0.52
1:E:18:LEU:HD23	1:E:26:PHE:CE1	2.45	0.52
1:A:35:PRO:HD3	1:A:58:GLY:O	2.08	0.52
1:E:18:LEU:HD21	1:E:25:PHE:CD2	2.45	0.51
1:E:46:ARG:HB3	1:E:183:ILE:HD11	1.92	0.51
1:B:141:ARG:CG	3:B:248:HOH:O	2.59	0.51
1:B:19:VAL:HG23	1:B:26:PHE:HE1	1.76	0.51
1:E:71:ILE:HG22	1:E:73:THR:H	1.75	0.51
1:A:25:PHE:CE2	1:A:26:PHE:CD2	2.97	0.50
1:A:150:ASN:O	1:A:154:GLN:HG2	2.12	0.49
1:E:18:LEU:HD21	1:E:25:PHE:CG	2.48	0.48
1:D:204:ARG:NE	3:D:264:HOH:O	2.46	0.48
1:D:36:ARG:NH1	1:D:91:GLU:OE1	2.46	0.48
1:E:44:ASP:O	1:E:45:SER:C	2.56	0.48
1:A:155:VAL:HG13	1:A:176:ILE:HG21	1.96	0.48
1:A:210:SER:O	1:A:214:LEU:HG	2.15	0.47
1:D:164:MET:HE1	1:D:174:VAL:HG11	1.96	0.47
1:A:19:VAL:O	1:A:19:VAL:CG1	2.56	0.47
1:B:214:LEU:O	1:B:215:LYS:C	2.58	0.47
1:A:37:PHE:CE2	1:B:4:ILE:CD1	2.95	0.47
1:E:132:SER:O	1:E:136:GLU:HG3	2.15	0.46
1:B:13:LEU:O	1:B:17:MET:HB2	2.15	0.46
1:D:24:GLY:HA2	1:D:27:GLU:HB2	1.97	0.46
1:E:47:VAL:HG12	1:E:52:LEU:HG	1.98	0.46
1:D:155:VAL:HG13	1:D:176:ILE:HG21	1.97	0.46
1:A:11:ASN:ND2	1:B:188:LEU:H	2.10	0.46
1:A:19:VAL:O	1:A:19:VAL:HG12	2.10	0.46
1:A:29:LEU:HB3	1:B:183:ILE:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LEU:HD23	1:D:124:ARG:HD3	1.98	0.45
1:D:41:GLY:C	1:D:68:ASN:HB3	2.42	0.45
1:B:71:ILE:O	1:B:72:HIS:C	2.58	0.45
1:E:98:HIS:CD2	1:E:101:CYS:HB2	2.52	0.45
1:A:22:ASP:O	1:A:23:PRO:C	2.59	0.44
1:B:193:VAL:HA	1:B:204:ARG:HB3	2.00	0.44
1:E:127:TRP:CE3	1:E:134:LEU:HD13	2.52	0.44
1:A:4:ILE:HD11	1:B:94:ILE:HD11	1.99	0.44
1:B:15:SER:O	1:B:16:LYS:C	2.53	0.44
1:D:46:ARG:HG2	1:D:98:HIS:CE1	2.53	0.44
1:A:126:ILE:HG12	1:A:153:GLU:HG3	2.00	0.44
1:A:67:ALA:C	1:A:68:ASN:CG	2.86	0.44
1:B:203:GLN:O	1:B:207:HIS:HD2	2.01	0.44
1:B:19:VAL:O	1:B:23:PRO:HD2	2.04	0.43
1:A:92:HIS:CG	1:B:4:ILE:HD11	2.53	0.43
1:A:17:MET:HE2	1:A:17:MET:C	2.43	0.43
1:E:150:ASN:O	1:E:154:GLN:HG2	2.19	0.43
1:E:155:VAL:HG13	1:E:176:ILE:HG21	1.99	0.43
1:B:18:LEU:O	1:B:23:PRO:HD3	2.19	0.43
1:A:36:ARG:O	1:A:36:ARG:HG2	2.19	0.43
1:E:60:LEU:HD23	1:E:60:LEU:H	1.83	0.43
1:A:117:ASN:O	1:A:121:LEU:HG	2.18	0.42
1:A:213:LYS:C	1:A:214:LEU:HD23	2.44	0.42
1:E:72:HIS:CE1	1:E:157:ASN:OD1	2.72	0.42
1:A:185:ASP:O	1:B:15:SER:OG	2.24	0.42
1:B:127:TRP:CD1	1:B:146:LEU:HD22	2.54	0.42
1:A:212:LEU:C	1:A:214:LEU:N	2.77	0.42
1:D:155:VAL:HG13	1:D:176:ILE:CG2	2.50	0.41
1:E:127:TRP:CZ3	1:E:134:LEU:HD13	2.55	0.41
1:D:181:TYR:HB3	1:D:188:LEU:HD23	2.02	0.41
1:A:76:ASN:HA	1:B:119:TRP:CZ3	2.56	0.41
1:B:130:HIS:CD2	1:B:149:LEU:HD22	2.55	0.41
1:B:152:MET:HG2	1:B:193:VAL:HG11	2.02	0.41
1:E:143:LEU:HD12	1:E:143:LEU:HA	1.91	0.41
1:D:33:GLN:HA	1:D:33:GLN:OE1	2.21	0.41
1:B:13:LEU:HD13	1:B:17:MET:SD	2.61	0.40
1:B:60:LEU:HD23	1:B:60:LEU:H	1.85	0.40
1:E:168:TRP:CD2	1:E:197:ASN:HA	2.56	0.40
1:B:141:ARG:HG2	3:B:248:HOH:O	2.19	0.40
1:D:164:MET:HE1	1:D:174:VAL:CG1	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:CD2	1:B:22:ASP:OD2[8_666]	1.92	0.28

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	212/220 (96%)	195 (92%)	14 (7%)	3 (1%)	9	17
1	B	212/220 (96%)	198 (93%)	14 (7%)	0	100	100
1	D	212/220 (96%)	201 (95%)	11 (5%)	0	100	100
1	E	212/220 (96%)	200 (94%)	12 (6%)	0	100	100
All	All	848/880 (96%)	794 (94%)	51 (6%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	23	PRO
1	A	67	ALA

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	187/192 (97%)	180 (96%)	7 (4%)	30	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	187/192 (97%)	178 (95%)	9 (5%)	23	46
1	D	187/192 (97%)	178 (95%)	9 (5%)	23	46
1	E	187/192 (97%)	175 (94%)	12 (6%)	16	33
All	All	748/768 (97%)	711 (95%)	37 (5%)	22	45

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	17	MET
1	A	20	GLU
1	A	23	PRO
1	A	66	VAL
1	A	75	LEU
1	A	131	SER
1	B	2	LYS
1	B	13	LEU
1	B	33	GLN
1	B	56	GLU
1	B	61	PHE
1	B	127	TRP
1	B	143	LEU
1	B	204	ARG
1	B	214	LEU
1	D	21	GLU
1	D	27	GLU
1	D	89	GLU
1	D	133	LEU
1	D	140	GLU
1	D	170	ARG
1	D	185	ASP
1	D	196	THR
1	D	203	GLN
1	E	20	GLU
1	E	21	GLU
1	E	28	LYS
1	E	131	SER
1	E	139	GLN
1	E	143	LEU
1	E	169	LYS
1	E	183	ILE

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Mol	Chain	Res	Type
1	E	193	VAL
1	E	198	ARG
1	E	204	ARG
1	E	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	11	ASN
1	A	110	ASN
1	A	160	HIS
1	B	105	GLN
1	B	117	ASN
1	B	207	HIS
1	D	10	ASN
1	D	110	ASN
1	E	33	GLN
1	E	110	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	15:SER	C	16:LYS	N	1.02

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	214/220 (97%)	0.17	4 (1%) 66 62	24, 39, 66, 77	0
1	B	214/220 (97%)	-0.06	12 (5%) 30 26	17, 29, 70, 73	0
1	D	214/220 (97%)	-0.10	2 (0%) 81 78	21, 35, 55, 69	0
1	E	214/220 (97%)	-0.20	4 (1%) 66 62	16, 28, 79, 89	0
All	All	856/880 (97%)	-0.05	22 (2%) 57 52	16, 33, 68, 89	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	ASP	6.1
1	A	25	PHE	3.8
1	E	19	VAL	3.5
1	B	17	MET	3.2
1	B	21	GLU	3.1
1	B	2	LYS	3.1
1	B	18	LEU	2.8
1	A	214	LEU	2.8
1	B	16	LYS	2.7
1	B	23	PRO	2.6
1	D	185	ASP	2.6
1	E	26	PHE	2.6
1	B	32	ALA	2.5
1	E	30	ALA	2.4
1	B	33	GLN	2.3
1	A	68	ASN	2.3
1	B	20	GLU	2.3
1	B	4	ILE	2.3
1	B	24	GLY	2.3
1	D	139	GLN	2.2
1	E	32	ALA	2.1
1	A	215	LYS	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($\text{\AA}^2$)	Q<0.9
2	ZN	D	221	1/1	0.99	0.02	39,39,39,39	0
2	ZN	B	221	1/1	1.00	0.02	34,34,34,34	0
2	ZN	A	221	1/1	1.00	0.02	40,40,40,40	0
2	ZN	E	221	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.