



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 12:32 AM EDT

PDB ID : 1C3B / pdb_00001c3b
Title : AMPC BETA-LACTAMASE FROM E. COLI COMPLEXED WITH INHIBITOR, BENZO(B)THIOPHENE-2-BORONIC ACID (BZB)
Authors : Powers, R.A.; Blazquez, J.; Weston, G.S.; Morosini, M.I.; Baquero, F.; Shoichet, B.K.
Deposited on : 1999-07-27
Resolution : 2.25 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

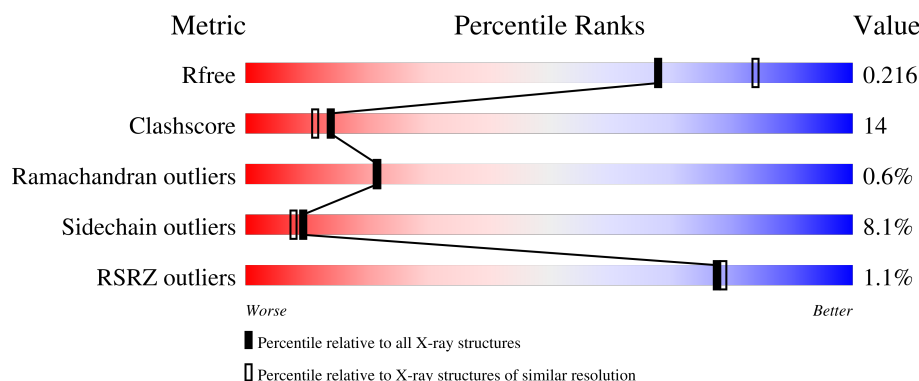
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.25 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}	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	358	 2% 66% 29% 5%
1	B	358	 69% 28%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BZB	A	362	-	-	X	-

2 Entry composition [i](#)

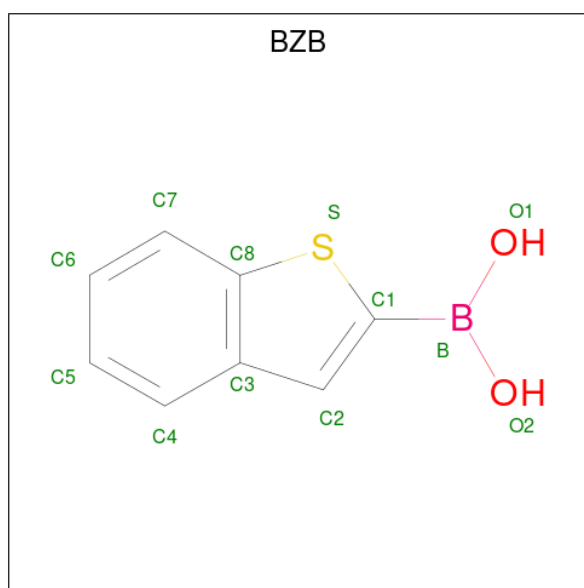
There are 3 unique types of molecules in this entry. The entry contains 5708 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CEPHALOSPORINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2795	1802	475	512	6			
1	B	358	Total	C	N	O	S	0	0	0
			2795	1802	475	512	6			

- Molecule 2 is BENZO[B]THIOPHENE-2-BORONIC ACID (CCD ID: BZB) (formula: $C_8H_7BO_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	O	S	0	0
			12	1	8	2	1		
2	B	1	Total	B	C	O	S	0	0
			12	1	8	2	1		

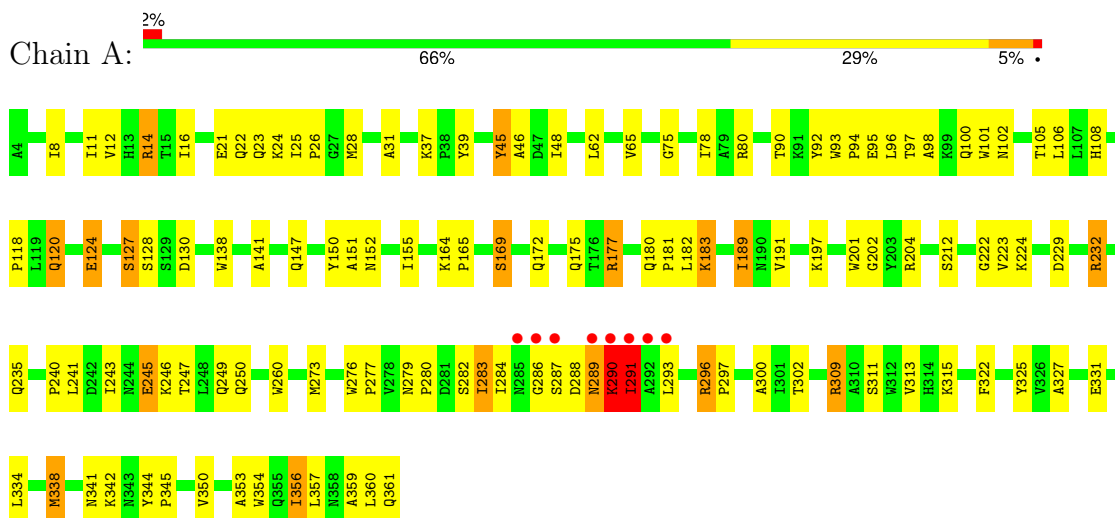
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total 43	O 43	0	0
3	B	51	Total 51	O 51	0	0

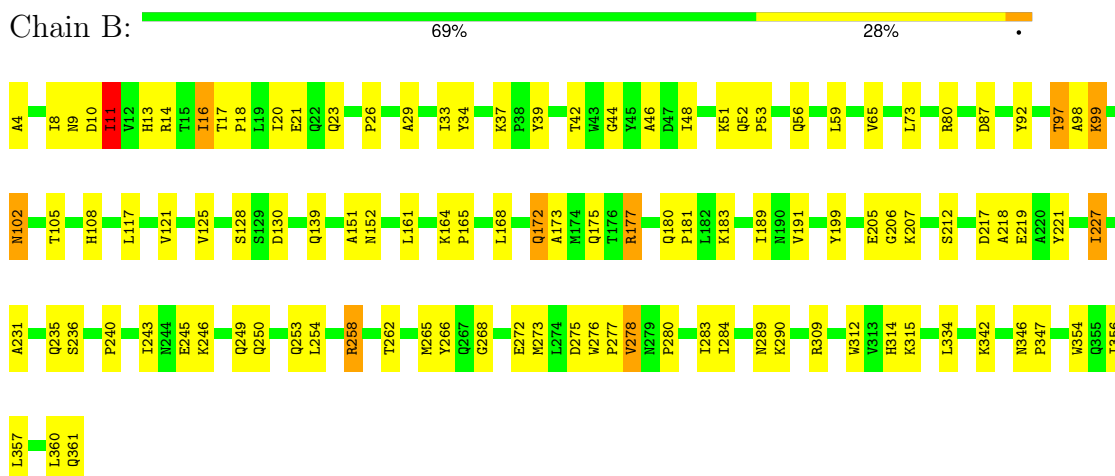
3 Residue-property plots

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: CEPHALOSPORINASE



• Molecule 1: CEPHALOSPORINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	118.86Å 78.01Å 98.96Å 90.00° 116.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 20.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	86.1 (20.00-2.25) 86.0 (20.00-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.58 (at 2.24Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.167 , 0.224 0.162 , 0.216	Depositor DCC
R_{free} test set	3304 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5708	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: BZB

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	0.69	2/2875 (0.1%)	1.05	15/3928 (0.4%)
1	B	0.63	0/2875	1.08	18/3928 (0.5%)
All	All	0.66	2/5750 (0.0%)	1.07	33/7856 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	LYS	N-CA	-6.43	1.37	1.46
1	A	338	MET	SD-CE	-5.11	1.66	1.79

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ILE	N-CA-C	-12.04	101.46	111.81
1	B	189	ILE	N-CA-C	-11.92	101.56	111.81
1	B	102	ASN	N-CA-C	7.83	120.58	111.02
1	B	16	ILE	N-CA-C	7.63	117.70	110.53
1	B	121	VAL	N-CA-C	-7.62	100.07	107.76
1	B	46	ALA	N-CA-C	-7.27	104.22	113.23
1	B	246	LYS	N-CA-C	6.69	118.22	111.07
1	B	128	SER	N-CA-C	-6.68	104.07	111.82
1	A	141	ALA	N-CA-C	-6.60	105.35	113.41
1	B	312	TRP	N-CA-C	-6.46	97.15	108.20
1	A	16	ILE	N-CA-C	6.44	117.23	110.72
1	A	45	TYR	N-CA-C	6.26	119.67	109.59
1	A	46	ALA	N-CA-C	-6.24	104.72	112.90
1	B	268	GLY	N-CA-C	-6.03	105.55	112.79
1	B	65	VAL	N-CA-C	-5.80	105.45	113.00
1	B	117	LEU	N-CA-C	-5.79	101.79	109.84
1	A	202	GLY	N-CA-C	-5.77	103.84	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	SER	N-CA-C	-5.64	102.93	110.55
1	A	356	ILE	N-CA-C	5.62	115.81	110.42
1	B	99	LYS	N-CA-C	5.61	118.93	111.75
1	B	11	ILE	CB-CA-C	-5.61	104.57	112.14
1	A	290	LYS	CA-CB-CG	-5.58	102.93	114.10
1	B	290	LYS	N-CA-C	-5.44	105.36	111.28
1	B	44	GLY	N-CA-C	5.38	121.59	111.80
1	A	118	PRO	N-CA-C	5.38	119.76	111.21
1	B	314	HIS	N-CA-C	5.36	115.62	108.38
1	A	151	ALA	N-CA-C	5.33	117.87	108.75
1	A	223	VAL	N-CA-C	5.33	116.45	109.21
1	B	73	LEU	N-CA-C	-5.27	105.53	111.28
1	A	291	ILE	CG1-CB-CG2	-5.22	95.03	110.70
1	B	151	ALA	N-CA-C	5.16	116.90	108.55
1	A	232	ARG	N-CA-C	-5.08	105.83	111.36
1	A	222	GLY	N-CA-C	5.04	123.53	115.66

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	2795	0	2771	90	0
1	B	2795	0	2771	68	0
2	A	12	0	7	4	0
2	B	12	0	7	1	0
3	A	43	0	0	0	0
3	B	51	0	0	4	0
All	All	5708	0	5556	157	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 14.

All (157) 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:296:ARG:HG3	1:A:296:ARG:HH11	1.13	1.12
1:A:14:ARG:HG3	1:A:14:ARG:HH11	0.98	1.09
1:A:11:ILE:HD11	1:A:356:ILE:HA	1.28	1.07
1:A:11:ILE:CD1	1:A:356:ILE:HA	2.01	0.91
1:A:14:ARG:HG3	1:A:14:ARG:NH1	1.78	0.91
1:B:56:GLN:HA	1:B:227:ILE:HD11	1.54	0.90
1:A:296:ARG:HH11	1:A:296:ARG:CG	1.89	0.85
1:A:11:ILE:HD12	1:A:359:ALA:HB3	1.57	0.84
1:A:94:PRO:HG2	1:A:95:GLU:OE1	1.76	0.84
1:B:168:LEU:HB3	1:B:172:GLN:HG2	1.61	0.83
1:A:280:PRO:O	1:A:284:ILE:HG13	1.79	0.83
1:A:14:ARG:HH11	1:A:14:ARG:CG	1.88	0.83
1:A:105:THR:H	1:A:108:HIS:CD2	1.98	0.82
1:B:29:ALA:HB1	1:B:227:ILE:HG12	1.62	0.81
1:A:241:LEU:HD11	1:B:250:GLN:HE21	1.46	0.81
1:B:105:THR:H	1:B:108:HIS:HD2	1.27	0.81
1:A:296:ARG:HG3	1:A:296:ARG:NH1	1.85	0.80
1:A:105:THR:H	1:A:108:HIS:HD2	1.30	0.79
1:B:265:MET:HE3	1:B:272:GLU:HG2	1.67	0.77
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.67	0.76
1:B:334:LEU:HG	1:B:357:LEU:HD22	1.68	0.74
1:A:240:PRO:HA	1:A:243:ILE:HD13	1.68	0.73
1:A:279:ASN:HB3	1:A:282:SER:HB2	1.71	0.72
1:A:338:MET:CE	1:A:353:ALA:HB2	2.20	0.72
1:A:245:GLU:CD	1:A:245:GLU:N	2.49	0.70
1:A:241:LEU:HD11	1:B:250:GLN:NE2	2.05	0.69
1:A:11:ILE:CD1	1:A:359:ALA:HB3	2.24	0.67
1:B:105:THR:H	1:B:108:HIS:CD2	2.11	0.67
1:A:338:MET:HE1	1:A:353:ALA:HB2	1.78	0.66
1:B:56:GLN:HA	1:B:227:ILE:CD1	2.26	0.65
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.77	0.65
1:B:11:ILE:HD11	1:B:360:LEU:HD21	1.79	0.63
1:A:124:GLU:H	1:A:124:GLU:CD	2.08	0.61
1:B:278:VAL:HG11	1:B:283:ILE:HD13	1.82	0.61
1:B:23:GLN:O	1:B:342:LYS:HE2	2.01	0.60
1:A:286:GLY:HA2	1:A:291:ILE:HG21	1.84	0.59
1:B:240:PRO:O	1:B:249:GLN:HG3	2.02	0.59
1:A:80:ARG:NH2	1:A:177:ARG:HG2	2.17	0.59
1:B:10:ASP:O	1:B:14:ARG:HG3	2.02	0.59
1:B:14:ARG:O	1:B:18:PRO:HG2	2.01	0.59
1:A:245:GLU:CD	1:A:245:GLU:H	2.09	0.58
1:A:11:ILE:HG23	1:A:12:VAL:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:HB2	1:B:165:PRO:HD3	1.87	0.57
1:A:120:GLN:HG2	2:A:362:BZB:HC51	1.86	0.57
1:A:325:TYR:HD2	1:A:338:MET:HE3	1.70	0.57
1:B:173:ALA:O	1:B:177:ARG:HB2	2.04	0.57
1:A:280:PRO:HG3	1:A:354:TRP:CE2	2.40	0.56
1:A:360:LEU:O	1:A:361:GLN:CB	2.53	0.56
1:B:258:ARG:NH2	1:B:275:ASP:OD2	2.31	0.56
1:A:147:GLN:HE21	1:A:297:PRO:N	2.04	0.56
1:A:344:TYR:HB2	1:A:345:PRO:HD2	1.87	0.56
1:B:59:LEU:HB2	1:B:199:TYR:HA	1.87	0.56
1:B:360:LEU:O	1:B:361:GLN:CB	2.54	0.54
1:B:180:GLN:HB2	1:B:181:PRO:HD3	1.89	0.54
1:A:11:ILE:HD11	1:A:356:ILE:CA	2.19	0.54
1:A:28:MET:HE3	1:A:338:MET:HB3	1.89	0.54
1:B:125:VAL:HG13	1:B:130:ASP:HB3	1.89	0.54
1:A:180:GLN:HB2	1:A:181:PRO:HD3	1.89	0.53
1:A:37:LYS:HD3	1:A:39:TYR:OH	2.08	0.53
1:B:250:GLN:O	1:B:254:LEU:HG	2.08	0.53
1:A:246:LYS:HG3	1:A:247:THR:H	1.73	0.53
1:A:152:ASN:HD21	2:A:362:BZB:C7	2.22	0.53
1:B:262:THR:O	1:B:262:THR:HG23	2.09	0.53
1:B:87:ASP:OD1	1:B:92:TYR:OH	2.22	0.52
1:A:98:ALA:HB3	1:A:101:TRP:HD1	1.75	0.52
1:A:8:ILE:O	1:A:11:ILE:HG22	2.11	0.51
1:A:240:PRO:O	1:A:249:GLN:HG3	2.10	0.51
1:A:150:TYR:CD1	1:A:293:LEU:HD22	2.45	0.51
1:A:280:PRO:O	1:A:283:ILE:HG13	2.10	0.51
1:B:168:LEU:HB3	1:B:172:GLN:CG	2.39	0.51
1:A:92:TYR:CE2	1:A:106:LEU:HD11	2.46	0.51
1:A:80:ARG:HH21	1:A:177:ARG:HG2	1.75	0.50
1:A:152:ASN:HD21	2:A:362:BZB:C8	2.25	0.49
1:A:246:LYS:HG3	1:A:247:THR:N	2.27	0.49
1:B:265:MET:HG2	1:B:266:TYR:N	2.26	0.49
1:B:80:ARG:NH2	1:B:177:ARG:HG2	2.27	0.49
1:B:280:PRO:HG3	1:B:354:TRP:CZ2	2.47	0.49
1:B:231:ALA:O	1:B:235:GLN:HG3	2.12	0.49
1:B:13:HIS:CD2	1:B:17:THR:OG1	2.65	0.49
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.48	0.49
1:A:287:SER:O	1:A:288:ASP:C	2.56	0.49
1:B:16:ILE:HG22	1:B:20:ILE:HD12	1.93	0.49
1:B:315:LYS:HE3	3:B:452:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLN:O	1:B:180:GLN:HG3	2.14	0.48
1:A:290:LYS:O	1:A:291:ILE:CB	2.61	0.48
1:A:243:ILE:HD12	1:A:243:ILE:N	2.29	0.47
1:B:258:ARG:HG3	1:B:273:MET:HE3	1.96	0.47
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.95	0.47
1:A:283:ILE:HB	1:A:350:VAL:HG11	1.96	0.47
1:A:182:LEU:O	1:A:183:LYS:HB2	2.12	0.47
1:B:53:PRO:HD2	3:B:456:HOH:O	2.14	0.47
1:A:105:THR:N	1:A:108:HIS:HD2	2.04	0.47
1:A:288:ASP:C	1:A:290:LYS:N	2.71	0.47
1:A:229:ASP:HA	1:A:232:ARG:HH11	1.80	0.46
1:A:11:ILE:CG2	1:A:12:VAL:N	2.78	0.46
1:B:161:LEU:HA	1:B:164:LYS:HG2	1.97	0.46
1:A:97:THR:O	1:A:98:ALA:C	2.58	0.46
1:B:280:PRO:O	1:B:284:ILE:HG13	2.15	0.46
1:A:201:TRP:O	1:A:341:ASN:HB2	2.15	0.46
1:B:52:GLN:HG2	3:B:456:HOH:O	2.16	0.46
1:B:258:ARG:HH22	1:B:275:ASP:CG	2.22	0.46
1:A:98:ALA:HB1	1:A:100:GLN:OE1	2.16	0.46
1:B:346:ASN:N	1:B:347:PRO:CD	2.79	0.46
1:B:29:ALA:HB1	1:B:227:ILE:CG1	2.41	0.45
1:A:75:GLY:HA2	1:A:78:ILE:HD12	1.99	0.45
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.51	0.45
1:A:313:VAL:O	1:A:327:ALA:HA	2.17	0.45
1:A:334:LEU:HG	1:A:357:LEU:HD22	1.99	0.45
1:B:33:ILE:HD12	1:B:33:ILE:N	2.31	0.45
1:A:93:TRP:O	1:A:96:LEU:HB2	2.17	0.45
1:A:90:THR:HG22	1:A:96:LEU:HB3	1.99	0.44
1:A:232:ARG:HA	1:A:235:GLN:HE21	1.82	0.44
1:B:17:THR:HB	1:B:18:PRO:HD3	1.98	0.44
1:B:152:ASN:HD21	2:B:362:BZB:C8	2.30	0.44
1:A:14:ARG:NH1	1:A:14:ARG:CG	2.58	0.44
1:B:265:MET:HE3	1:B:272:GLU:CG	2.43	0.44
1:B:276:TRP:HA	1:B:277:PRO:C	2.43	0.44
1:B:17:THR:O	1:B:21:GLU:HG2	2.17	0.44
1:B:227:ILE:HG13	3:B:412:HOH:O	2.18	0.44
1:A:31:ALA:HA	1:A:39:TYR:O	2.18	0.44
1:A:290:LYS:O	1:A:291:ILE:HG13	2.17	0.43
1:A:309:ARG:O	1:A:331:GLU:HB2	2.18	0.43
1:A:309:ARG:HH21	1:A:331:GLU:CG	2.31	0.43
1:A:169:SER:OG	1:A:172:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HG22	1:B:20:ILE:CD1	2.49	0.43
1:A:289:ASN:HD22	1:A:289:ASN:HA	1.69	0.43
1:A:322:PHE:CD2	1:A:341:ASN:HA	2.53	0.43
1:B:205:GLU:C	1:B:207:LYS:H	2.26	0.43
1:A:23:GLN:HB2	1:A:25:ILE:HG13	2.01	0.42
1:B:16:ILE:HD11	1:B:356:ILE:HD11	2.00	0.42
1:A:164:LYS:O	1:A:165:PRO:C	2.62	0.42
1:A:45:TYR:N	1:A:45:TYR:CD2	2.87	0.42
1:A:127:SER:O	1:A:130:ASP:HB2	2.20	0.42
1:A:243:ILE:N	1:A:243:ILE:CD1	2.83	0.42
1:B:16:ILE:HD13	1:B:16:ILE:N	2.34	0.42
1:A:344:TYR:HB2	1:A:345:PRO:CD	2.50	0.41
1:B:273:MET:HE2	1:B:273:MET:HB2	1.86	0.41
1:A:100:GLN:NE2	1:A:138:TRP:O	2.53	0.41
2:A:362:BZB:HO21	2:A:362:BZB:C1	2.28	0.41
1:B:219:GLU:OE1	1:B:219:GLU:N	2.52	0.41
1:A:11:ILE:HD12	1:A:359:ALA:CB	2.41	0.41
1:A:288:ASP:C	1:A:290:LYS:H	2.27	0.41
1:B:97:THR:O	1:B:98:ALA:C	2.64	0.41
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.55	0.41
1:A:23:GLN:O	1:A:24:LYS:HB2	2.20	0.41
1:A:246:LYS:HG3	1:A:247:THR:HG23	2.02	0.41
1:B:8:ILE:HD11	1:B:34:TYR:CG	2.56	0.41
1:B:249:GLN:O	1:B:253:GLN:HG3	2.21	0.41
1:B:125:VAL:HG13	1:B:130:ASP:C	2.46	0.41
1:B:217:ASP:OD1	1:B:218:ALA:N	2.53	0.41
1:B:181:PRO:HB3	1:B:245:GLU:HG3	2.02	0.41
1:B:139:GLN:NE2	1:B:139:GLN:HA	2.35	0.40
1:B:236:SER:HB3	1:B:243:ILE:HD11	2.03	0.40
1:A:260:TRP:CZ3	1:A:300:ALA:HB2	2.56	0.40
1:A:62:LEU:HB3	1:A:65:VAL:HB	2.03	0.40
1:B:4:ALA:HB2	1:B:39:TYR:CD1	2.56	0.40
1:B:289:ASN:HD22	1:B:289:ASN:HA	1.67	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	356/358 (99%)	342 (96%)	12 (3%)	2 (1%)	22	21
1	B	356/358 (99%)	347 (98%)	7 (2%)	2 (1%)	22	21
All	All	712/716 (99%)	689 (97%)	19 (3%)	4 (1%)	22	21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ILE
1	A	102	ASN
1	B	206	GLY
1	B	221	TYR

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	291/292 (100%)	261 (90%)	30 (10%)	6	4
1	B	291/292 (100%)	274 (94%)	17 (6%)	17	16
All	All	582/584 (100%)	535 (92%)	47 (8%)	9	8

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	21	GLU

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Mol	Chain	Res	Type
1	A	22	GLN
1	A	120	GLN
1	A	124	GLU
1	A	127	SER
1	A	128	SER
1	A	155	ILE
1	A	175	GLN
1	A	177	ARG
1	A	183	LYS
1	A	189	ILE
1	A	191	VAL
1	A	197	LYS
1	A	204	ARG
1	A	212	SER
1	A	224	LYS
1	A	245	GLU
1	A	250	GLN
1	A	273	MET
1	A	283	ILE
1	A	289	ASN
1	A	290	LYS
1	A	291	ILE
1	A	296	ARG
1	A	302	THR
1	A	309	ARG
1	A	311	SER
1	A	315	LYS
1	A	342	LYS
1	B	9	ASN
1	B	11	ILE
1	B	37	LYS
1	B	42	THR
1	B	51	LYS
1	B	97	THR
1	B	99	LYS
1	B	102	ASN
1	B	172	GLN
1	B	177	ARG
1	B	183	LYS
1	B	191	VAL
1	B	212	SER
1	B	227	ILE

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Mol	Chain	Res	Type
1	B	258	ARG
1	B	278	VAL
1	B	309	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	23	GLN
1	A	108	HIS
1	A	137	ASN
1	A	147	GLN
1	A	190	ASN
1	A	235	GLN
1	A	253	GLN
1	B	9	ASN
1	B	13	HIS
1	B	22	GLN
1	B	23	GLN
1	B	108	HIS
1	B	137	ASN
1	B	139	GLN
1	B	249	GLN
1	B	253	GLN
1	B	285	ASN
1	B	289	ASN
1	B	358	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	BZB	A	362	1	11,13,13	3.13	3 (27%)	8,18,18	2.94	2 (25%)
2	BZB	B	362	1	11,13,13	2.63	4 (36%)	8,18,18	2.92	2 (25%)

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	BZB	A	362	1	-	0/0/4/4	0/2/2/2
2	BZB	B	362	1	-	0/0/4/4	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	362	BZB	B-O1	8.39	1.50	1.36
2	B	362	BZB	B-O1	6.95	1.47	1.36
2	A	362	BZB	B-O2	4.29	1.43	1.36
2	B	362	BZB	C5-C4	2.79	1.42	1.36
2	B	362	BZB	B-O2	2.62	1.40	1.36
2	A	362	BZB	C5-C4	2.59	1.42	1.36
2	B	362	BZB	C7-C8	2.19	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	362	BZB	O2-B-C1	-6.11	101.94	120.56
2	A	362	BZB	O2-B-C1	-6.07	102.05	120.56
2	A	362	BZB	O1-B-C1	-5.43	104.00	120.56
2	B	362	BZB	O1-B-C1	-5.26	104.54	120.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	362	BZB	4	0
2	B	362	BZB	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	358/358 (100%)	-0.39	8 (2%) 62 62	9, 22, 54, 84	0
1	B	358/358 (100%)	-0.48	0 100 100	10, 24, 45, 65	0
All	All	716/716 (100%)	-0.43	8 (1%) 77 79	9, 23, 48, 84	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	GLY	7.0
1	A	292	ALA	4.3
1	A	290	LYS	4.1
1	A	291	ILE	3.8
1	A	287	SER	3.6
1	A	293	LEU	3.2
1	A	285	ASN	2.3
1	A	289	ASN	2.1

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, 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(\AA^2)	Q<0.9
2	BZB	A	362	12/12	0.89	0.11	19,31,35,35	0
2	BZB	B	362	12/12	0.90	0.10	15,25,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.