



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:45 PM GMT

PDB ID : 1CBX
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN CARBOXYPEPTIDASE A AND THE BIPRODUCT ANALOG INHIBITOR L-BENZYL SUCCINATE AT 2.0 ANGSTROMS RESOLUTION
Authors : Mangani, S.; Carloni, P.; Orioli, P.
Deposited on : 1991-10-31
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

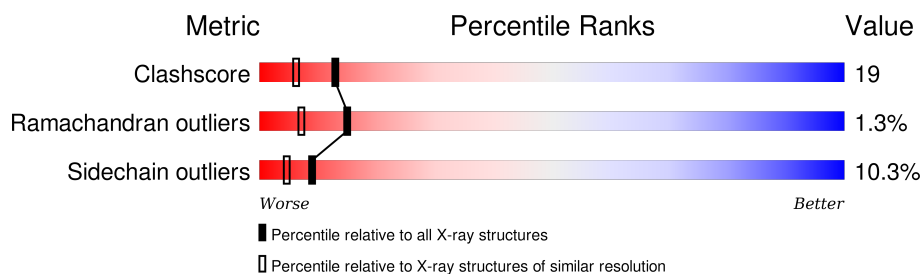
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	 49% 36% 12% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2631 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

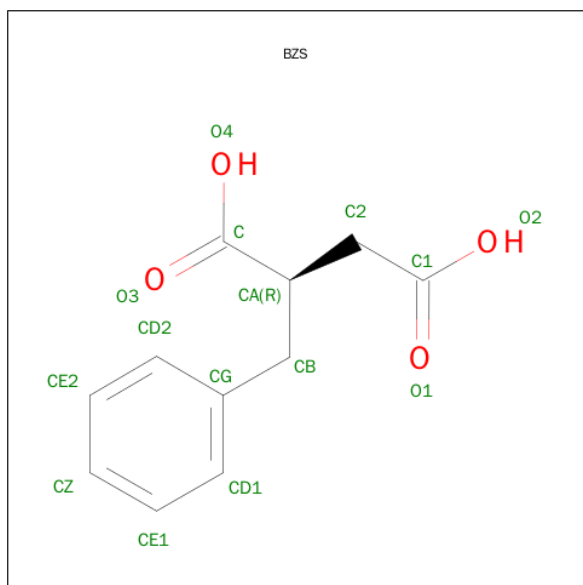
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASN	ASP	CONFLICT	UNP P00730
A	93	ASN	ASP	CONFLICT	UNP P00730
A	114	ASN	ASP	CONFLICT	UNP P00730
A	122	GLU	GLN	CONFLICT	UNP P00730
A	185	ASN	ASP	CONFLICT	UNP P00730
A	228	ALA	GLU	CONFLICT	UNP P00730
A	305	VAL	LEU	CONFLICT	UNP P00730

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

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

- Molecule 3 is L-BENZYL SUCCINIC ACID (three-letter code: BZS) (formula: C₁₁H₁₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			15	11	4		

- Molecule 4 is water.

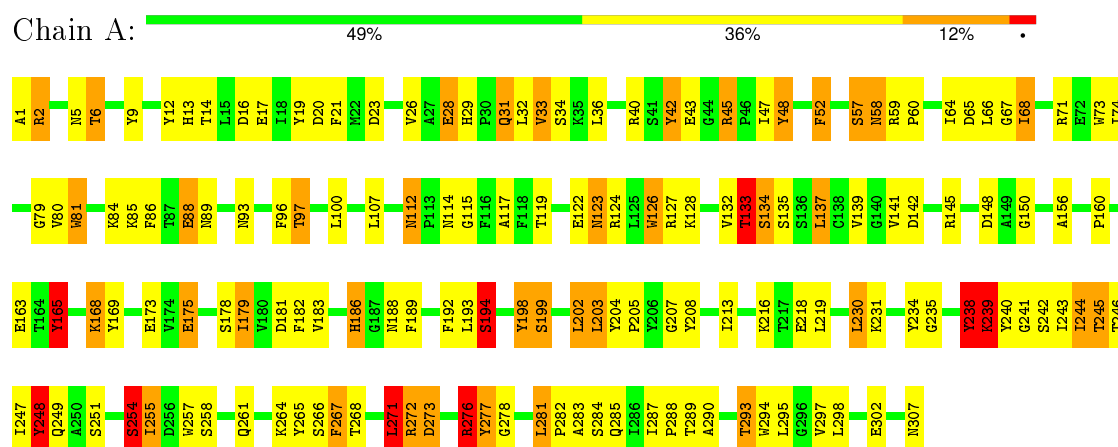
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	178	Total	O	0	0
			178	178		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: CARBOXYPEPTIDASE A



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.60Å 60.27Å 47.25Å 90.00° 97.27° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2631	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.72	25/2503 (1.0%)	2.13	90/3402 (2.6%)

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	A	0	13

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	43	GLU	CD-OE1	9.99	1.36	1.25
1	A	122	GLU	CD-OE1	8.57	1.35	1.25
1	A	218	GLU	CD-OE2	7.83	1.34	1.25
1	A	173	GLU	CD-OE2	7.50	1.33	1.25
1	A	88	GLU	CD-OE2	-7.32	1.17	1.25
1	A	17	GLU	CD-OE2	7.06	1.33	1.25
1	A	40	ARG	CZ-NH1	6.94	1.42	1.33
1	A	178	SER	CB-OG	6.76	1.51	1.42
1	A	302	GLU	CD-OE2	6.59	1.32	1.25
1	A	271	LEU	C-O	6.54	1.35	1.23
1	A	163	GLU	CD-OE1	6.38	1.32	1.25
1	A	175	GLU	CD-OE2	6.24	1.32	1.25
1	A	254	SER	CB-OG	-6.12	1.34	1.42
1	A	238	TYR	CZ-OH	-6.02	1.27	1.37
1	A	17	GLU	CD-OE1	-5.85	1.19	1.25
1	A	66	LEU	C-N	-5.67	1.22	1.33
1	A	73	TRP	CD2-CE3	-5.65	1.31	1.40
1	A	183	VAL	C-N	5.59	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	GLY	C-O	-5.58	1.14	1.23
1	A	183	VAL	C-O	5.42	1.33	1.23
1	A	276	ARG	C-O	5.37	1.33	1.23
1	A	28	GLU	CD-OE2	5.32	1.31	1.25
1	A	145	ARG	CZ-NH1	5.32	1.40	1.33
1	A	254	SER	C-O	5.25	1.33	1.23
1	A	182	PHE	CB-CG	5.23	1.60	1.51

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ARG	NE-CZ-NH2	-18.61	111.00	120.30
1	A	248	TYR	CB-CG-CD2	13.45	129.07	121.00
1	A	142	ASP	CB-CG-OD2	-12.76	106.82	118.30
1	A	248	TYR	CB-CG-CD1	-12.52	113.49	121.00
1	A	40	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	A	16	ASP	CB-CG-OD1	11.40	128.56	118.30
1	A	182	PHE	CB-CG-CD1	-11.29	112.90	120.80
1	A	145	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	A	277	TYR	CB-CG-CD2	-11.24	114.26	121.00
1	A	42	TYR	CB-CG-CD1	-10.71	114.57	121.00
1	A	20	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	208	TYR	CB-CG-CD1	10.47	127.28	121.00
1	A	142	ASP	CB-CG-OD1	10.08	127.37	118.30
1	A	148	ASP	CB-CG-OD1	8.95	126.36	118.30
1	A	20	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	9	TYR	CG-CD2-CE2	-8.66	114.37	121.30
1	A	48	TYR	CB-CG-CD1	8.35	126.01	121.00
1	A	255	ILE	CA-CB-CG2	8.30	127.51	110.90
1	A	16	ASP	CB-CG-OD2	-8.26	110.86	118.30
1	A	71	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	277	TYR	CB-CG-CD1	7.95	125.77	121.00
1	A	45	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	9	TYR	CG-CD1-CE1	7.80	127.54	121.30
1	A	273	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	9	TYR	CD1-CE1-CZ	-7.45	113.10	119.80
1	A	182	PHE	CB-CG-CD2	7.45	126.01	120.80
1	A	127	ARG	NE-CZ-NH2	7.45	124.02	120.30
1	A	272	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	48	TYR	CG-CD2-CE2	7.34	127.17	121.30
1	A	165	TYR	CB-CG-CD1	-7.28	116.63	121.00
1	A	208	TYR	CB-CG-CD2	-6.94	116.84	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	2	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	119	THR	CA-C-O	-6.60	106.23	120.10
1	A	181	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	169	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	A	202	LEU	CB-CA-C	-6.38	98.09	110.20
1	A	48	TYR	O-C-N	6.32	132.82	122.70
1	A	48	TYR	CB-CG-CD2	-6.31	117.21	121.00
1	A	148	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	9	TYR	CZ-CE2-CD2	6.30	125.47	119.80
1	A	48	TYR	CD1-CE1-CZ	6.25	125.42	119.80
1	A	65	ASP	N-CA-CB	6.24	121.84	110.60
1	A	165	TYR	CD1-CE1-CZ	-6.15	114.26	119.80
1	A	194	SER	N-CA-CB	6.12	119.69	110.50
1	A	48	TYR	CG-CD1-CE1	-6.09	116.42	121.30
1	A	254	SER	N-CA-CB	-6.08	101.39	110.50
1	A	133	THR	O-C-N	6.04	132.36	122.70
1	A	122	GLU	O-C-N	-5.99	113.12	122.70
1	A	80	VAL	CG1-CB-CG2	-5.85	101.55	110.90
1	A	202	LEU	N-CA-CB	5.84	122.09	110.40
1	A	141	VAL	CG1-CB-CG2	-5.83	101.58	110.90
1	A	40	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	248	TYR	CA-CB-CG	5.78	124.39	113.40
1	A	234	TYR	CZ-CE2-CD2	-5.76	114.61	119.80
1	A	234	TYR	CG-CD2-CE2	5.76	125.91	121.30
1	A	122	GLU	CG-CD-OE1	-5.73	106.85	118.30
1	A	14	THR	CA-CB-CG2	-5.71	104.41	112.40
1	A	238	TYR	CZ-CE2-CD2	-5.65	114.72	119.80
1	A	244	ILE	CA-CB-CG2	5.63	122.16	110.90
1	A	281	LEU	CB-CG-CD2	5.62	120.56	111.00
1	A	297	VAL	CG1-CB-CG2	5.58	119.83	110.90
1	A	52	PHE	CZ-CE2-CD2	5.56	126.78	120.10
1	A	124	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	240	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	267	PHE	CB-CG-CD1	5.47	124.63	120.80
1	A	239	LYS	N-CA-CB	5.47	120.44	110.60
1	A	126	TRP	C-N-CA	5.45	135.33	121.70
1	A	124	ARG	CA-C-O	5.44	131.53	120.10
1	A	183	VAL	CG1-CB-CG2	5.41	119.56	110.90
1	A	163	GLU	O-C-N	-5.37	114.11	122.70
1	A	17	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	258	SER	CB-CA-C	5.33	120.22	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	ALA	CA-C-O	5.28	131.19	120.10
1	A	182	PHE	N-CA-CB	-5.27	101.11	110.60
1	A	123	ASN	N-CA-CB	-5.25	101.15	110.60
1	A	81	TRP	CE3-CZ3-CH2	-5.20	115.48	121.20
1	A	165	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	265	TYR	CG-CD2-CE2	5.18	125.44	121.30
1	A	255	ILE	CB-CA-C	5.18	121.95	111.60
1	A	122	GLU	OE1-CD-OE2	5.17	129.51	123.30
1	A	165	TYR	CZ-CE2-CD2	-5.17	115.15	119.80
1	A	267	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	68	ILE	CG1-CB-CG2	-5.16	100.05	111.40
1	A	234	TYR	CB-CG-CD2	5.11	124.07	121.00
1	A	12	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	238	TYR	CB-CG-CD1	-5.07	117.96	121.00
1	A	23	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	A	186	HIS	N-CA-CB	-5.02	101.56	110.60
1	A	13	HIS	CA-CB-CG	-5.01	105.09	113.60

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	156	ALA	Mainchain
1	A	165	TYR	Sidechain
1	A	189	PHE	Sidechain
1	A	19	TYR	Sidechain
1	A	198	TYR	Peptide
1	A	203	LEU	Mainchain
1	A	21	PHE	Sidechain
1	A	230	LEU	Mainchain
1	A	238	TYR	Sidechain
1	A	278	GLY	Mainchain
1	A	283	ALA	Mainchain
1	A	47	ILE	Mainchain
1	A	58	ASN	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	2437	0	2351	92	0
2	A	1	0	0	0	0
3	A	15	0	10	0	0
4	A	178	0	0	12	0
All	All	2631	0	2361	92	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 19.

All (92) 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:289:THR:O	1:A:293:THR:HG23	1.37	1.24
1:A:137:LEU:HD22	1:A:137:LEU:H	1.16	1.04
1:A:289:THR:O	1:A:293:THR:CG2	2.15	0.94
1:A:137:LEU:HD22	1:A:137:LEU:N	1.96	0.81
1:A:31:GLN:HB2	4:A:588:HOH:O	1.84	0.77
1:A:175:GLU:O	1:A:179:ILE:HD13	1.85	0.76
1:A:254:SER:OG	4:A:648:HOH:O	2.04	0.73
1:A:186:HIS:HD2	1:A:188:ASN:H	1.37	0.72
1:A:86:PHE:HE1	1:A:294:TRP:CZ3	2.08	0.72
1:A:85:LYS:HE3	1:A:89:ASN:ND2	2.07	0.70
1:A:207:GLY:O	1:A:249:GLN:CG	2.40	0.70
1:A:133:THR:O	1:A:134:SER:HB3	1.91	0.69
1:A:168:LYS:HG2	4:A:547:HOH:O	1.94	0.68
1:A:45:ARG:HH11	1:A:114:ASN:ND2	1.92	0.68
1:A:179:ILE:N	1:A:179:ILE:HD12	2.10	0.67
1:A:137:LEU:CD2	1:A:137:LEU:H	2.00	0.66
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.26	0.66
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.61	0.65
1:A:242:SER:OG	1:A:245:THR:HB	1.97	0.64
1:A:134:SER:OG	1:A:135:SER:N	2.29	0.64
1:A:207:GLY:O	1:A:249:GLN:HG3	1.96	0.64
1:A:45:ARG:HH11	1:A:114:ASN:HD22	1.44	0.63
1:A:45:ARG:HD2	1:A:114:ASN:HD22	1.62	0.63
1:A:42:TYR:OH	1:A:132:VAL:HG22	1.99	0.61
1:A:245:THR:HG21	4:A:539:HOH:O	2.02	0.60
1:A:26:VAL:HG22	1:A:33:VAL:HG22	1.83	0.59
1:A:207:GLY:O	1:A:249:GLN:HG2	2.03	0.59
1:A:179:ILE:N	1:A:179:ILE:CD1	2.64	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASN:ND2	1:A:188:ASN:HB2	2.18	0.57
1:A:239:LYS:HE3	4:A:668:HOH:O	2.05	0.56
1:A:244:ILE:HD12	1:A:249:GLN:HG3	1.88	0.55
1:A:93:ASN:O	1:A:97:THR:CG2	2.54	0.55
1:A:93:ASN:O	1:A:97:THR:HG23	2.08	0.53
1:A:175:GLU:O	1:A:179:ILE:CD1	2.55	0.53
1:A:230:LEU:C	1:A:230:LEU:HD23	2.30	0.53
1:A:186:HIS:HE1	4:A:612:HOH:O	1.92	0.52
1:A:230:LEU:HD23	1:A:230:LEU:O	2.09	0.52
1:A:241:GLY:HA3	1:A:246:THR:OG1	2.10	0.52
1:A:287:ILE:N	1:A:288:PRO:HD2	2.26	0.51
1:A:112:ASN:ND2	1:A:115:GLY:H	2.08	0.51
1:A:254:SER:CB	4:A:661:HOH:O	2.58	0.51
1:A:257:TRP:O	1:A:261:GLN:HG2	2.10	0.51
1:A:32:LEU:HD11	1:A:100:LEU:HD13	1.92	0.50
1:A:254:SER:HB2	4:A:661:HOH:O	2.12	0.50
1:A:204:TYR:HB2	1:A:205:PRO:HD2	1.92	0.50
1:A:239:LYS:CE	4:A:668:HOH:O	2.60	0.48
1:A:186:HIS:HD2	1:A:188:ASN:N	2.10	0.47
1:A:192:PHE:O	1:A:193:LEU:HD12	2.14	0.47
1:A:179:ILE:H	1:A:179:ILE:CD1	2.28	0.47
1:A:88:GLU:OE1	4:A:584:HOH:O	2.20	0.47
1:A:32:LEU:O	1:A:52:PHE:HA	2.15	0.46
1:A:272:ARG:HB3	1:A:273:ASP:HA	1.97	0.46
1:A:238:TYR:OH	1:A:271:LEU:HA	2.15	0.46
1:A:1:ALA:N	1:A:6:THR:HG22	2.30	0.46
1:A:272:ARG:HH11	1:A:285:GLN:HE21	1.62	0.46
1:A:6:THR:HG21	4:A:600:HOH:O	2.15	0.46
1:A:45:ARG:HD2	1:A:114:ASN:ND2	2.29	0.46
1:A:231:LYS:O	1:A:235:GLY:HA2	2.16	0.46
1:A:276:ARG:C	1:A:276:ARG:HD3	2.35	0.45
1:A:132:VAL:HG23	1:A:133:THR:OG1	2.16	0.45
1:A:204:TYR:O	1:A:242:SER:HA	2.17	0.45
1:A:133:THR:O	1:A:134:SER:CB	2.63	0.45
1:A:255:ILE:HD12	1:A:266:SER:HB3	1.98	0.44
1:A:160:PRO:HA	1:A:165:TYR:CD2	2.52	0.44
1:A:276:ARG:HD2	1:A:277:TYR:CE2	2.52	0.44
1:A:68:ILE:HG21	1:A:68:ILE:HD13	1.74	0.43
1:A:264:LYS:HG2	1:A:264:LYS:O	2.17	0.43
1:A:28:GLU:C	1:A:29:HIS:CG	2.91	0.43
1:A:126:TRP:NE1	1:A:128:LYS:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASN:ND2	1:A:96:PHE:H	2.17	0.43
1:A:247:ILE:HG12	1:A:248:TYR:CD2	2.54	0.43
1:A:194:SER:O	1:A:268:THR:HG23	2.18	0.43
1:A:204:TYR:CB	1:A:205:PRO:CD	2.94	0.43
1:A:93:ASN:O	1:A:97:THR:HG22	2.18	0.43
1:A:2:ARG:H	1:A:6:THR:HG21	1.83	0.43
1:A:36:LEU:O	1:A:48:TYR:HA	2.19	0.43
1:A:276:ARG:O	1:A:276:ARG:HD3	2.19	0.42
1:A:150:GLY:O	1:A:251:SER:HB2	2.19	0.42
1:A:219:LEU:HG	1:A:267:PHE:CZ	2.55	0.42
1:A:123:ASN:OD1	1:A:123:ASN:C	2.56	0.42
1:A:192:PHE:HD1	1:A:255:ILE:CD1	2.33	0.42
1:A:213:ILE:HD12	1:A:219:LEU:HD22	2.02	0.42
1:A:198:TYR:O	1:A:199:SER:CB	2.67	0.41
1:A:64:ILE:HB	1:A:107:LEU:HD12	2.01	0.41
1:A:186:HIS:CD2	1:A:188:ASN:H	2.26	0.41
1:A:207:GLY:HA2	1:A:243:ILE:HB	2.03	0.41
1:A:5:ASN:HD21	1:A:84:LYS:HZ1	1.69	0.41
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.75	0.40
1:A:67:GLY:O	4:A:529:HOH:O	2.21	0.40
1:A:81:TRP:CE3	1:A:290:ALA:HB1	2.57	0.40
1:A:60:PRO:HA	1:A:188:ASN:O	2.21	0.40
1:A:282:PRO:C	1:A:284:SER:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	305/307 (99%)	287 (94%)	14 (5%)	4 (1%)	15 7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	THR
1	A	134	SER
1	A	199	SER
1	A	57	SER

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	263/263 (100%)	236 (90%)	27 (10%)	9 5

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	31	GLN
1	A	33	VAL
1	A	34	SER
1	A	57	SER
1	A	74	ILE
1	A	97	THR
1	A	112	ASN
1	A	137	LEU
1	A	139	VAL
1	A	168	LYS
1	A	179	ILE
1	A	194	SER
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	239	LYS
1	A	245	THR
1	A	248	TYR
1	A	254	SER
1	A	271	LEU
1	A	276	ARG
1	A	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	THR
1	A	295	LEU
1	A	298	LEU
1	A	307	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	37	GLN
1	A	58	ASN
1	A	89	ASN
1	A	93	ASN
1	A	112	ASN
1	A	114	ASN
1	A	171	ASN
1	A	186	HIS
1	A	285	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	BZS	A	500	2	9,15,15	1.49	2 (22%)	12,19,19	3.29	3 (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
3	BZS	A	500	2	-	0/6/12/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	BZS	CE2-CD2	-2.13	1.34	1.38
3	A	500	BZS	CB-CG	2.58	1.57	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	BZS	CG-CB-CA	-9.77	99.77	113.92
3	A	500	BZS	C1-C2-CA	-4.52	106.84	113.87
3	A	500	BZS	CB-CA-C	-2.60	105.94	111.03

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.