



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:41 PM UTC

PDB ID : 3O9M / pdb_00003o9m
Title : Co-crystallization studies of full length recombinant BChE with cocaine offers insights into cocaine detoxification
Authors : Asojo, O.A.; Ngamelue, M.N.; Homma, K.; Lockridge, O.
Deposited on : 2010-08-04
Resolution : 2.98 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

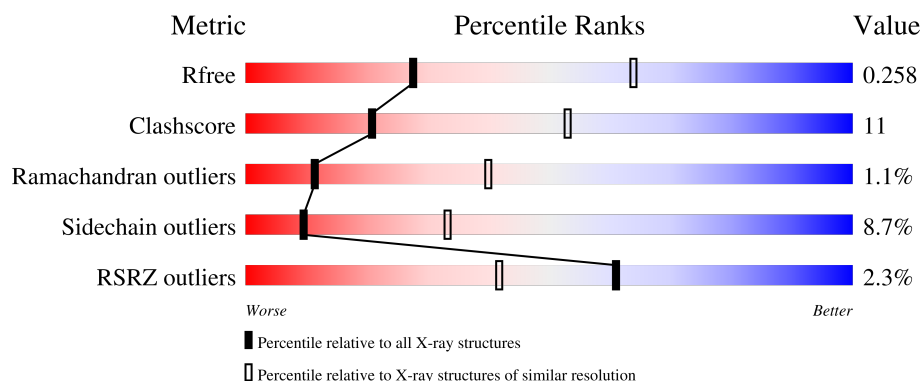
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

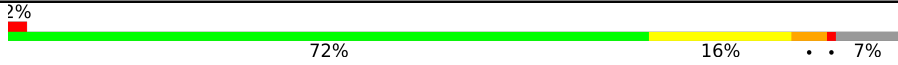
The reported resolution of this entry is 2.98 Å.

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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	574	
1	B	574	

2 Entry composition [i](#)

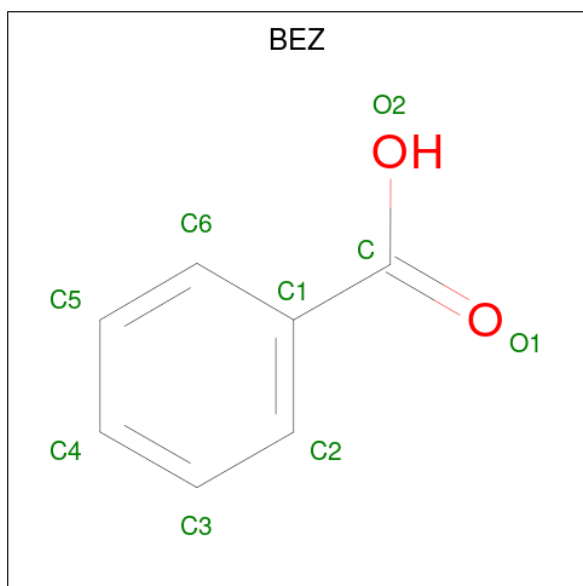
There are 3 unique types of molecules in this entry. The entry contains 8472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4226	2726	710	774	16			
1	B	531	Total	C	N	O	S	0	0	0
			4226	2726	710	774	16			

- Molecule 2 is BENZOIC ACID (CCD ID: BEZ) (formula: $C_7H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	7	2		
2	B	1	Total	C	O	0	0
			9	7	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	O 1	0	0
3	B	1	Total 1	O 1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	150.39Å 150.39Å 142.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	142.45 – 2.98 142.45 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.7 (142.45-2.98) 99.7 (142.45-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.22 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.262 0.217 , 0.258	Depositor DCC
R_{free} test set	1720 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8472	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.96% 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: BEZ

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	1.04	6/4345 (0.1%)	1.18	16/5900 (0.3%)
1	B	0.99	5/4345 (0.1%)	1.13	16/5900 (0.3%)
All	All	1.02	11/8690 (0.1%)	1.15	32/11800 (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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ALA	C-O	-12.42	1.13	1.24
1	A	101	ALA	CA-C	-7.30	1.44	1.52
1	A	40	ARG	CZ-NH2	6.96	1.42	1.33
1	A	105	LYS	CA-C	6.84	1.58	1.52
1	B	101	ALA	C-O	-6.62	1.16	1.24
1	A	488	THR	CA-CB	5.57	1.62	1.53
1	A	364	PHE	CB-CG	-5.50	1.38	1.50
1	B	105	LYS	CD-CE	5.47	1.68	1.52
1	B	40	ARG	CZ-NH2	-5.37	1.26	1.33
1	B	488	THR	CA-CB	5.23	1.62	1.53
1	B	5	ILE	CA-CB	5.20	1.61	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ALA	CA-C-N	-18.16	97.15	119.84
1	A	101	ALA	C-N-CA	-18.16	97.15	119.84
1	A	413	GLY	N-CA-C	9.01	124.33	113.79
1	A	105	LYS	CB-CA-C	8.65	124.50	110.83
1	A	101	ALA	CA-C-O	-8.59	110.92	119.08
1	B	104	PRO	CA-C-N	8.58	137.93	121.54
1	B	104	PRO	C-N-CA	8.58	137.93	121.54
1	B	291	GLY	CA-C-N	7.72	127.71	119.76
1	B	291	GLY	C-N-CA	7.72	127.71	119.76
1	A	291	GLY	CA-C-N	7.51	127.56	119.90
1	A	291	GLY	C-N-CA	7.51	127.56	119.90
1	B	441	GLU	N-CA-C	-6.93	104.97	113.50
1	A	481	ASN	CB-CA-C	6.63	120.75	109.80
1	B	413	GLY	N-CA-C	6.56	121.47	113.79
1	A	101	ALA	N-CA-C	6.49	121.31	112.55
1	B	364	PHE	N-CA-CB	-6.43	100.61	110.13
1	A	484	GLN	N-CA-C	6.39	118.13	111.03
1	B	104	PRO	O-C-N	-6.36	115.24	123.00
1	A	507	SER	N-CA-C	6.17	121.49	111.37
1	B	104	PRO	N-CA-C	-5.94	102.50	111.41
1	B	400	CYS	CA-C-N	-5.73	112.69	119.05
1	B	400	CYS	C-N-CA	-5.73	112.69	119.05
1	A	483	THR	N-CA-C	5.51	118.21	111.82
1	B	481	ASN	CB-CA-C	5.42	119.32	109.83
1	B	101	ALA	C-N-CD	-5.38	108.77	120.60
1	A	302	MET	CB-CG-SD	5.21	128.32	112.70
1	A	255	GLU	N-CA-C	-5.19	103.61	111.34
1	A	364	PHE	CB-CA-C	-5.18	102.09	110.79
1	A	392	VAL	N-CA-C	-5.18	105.45	110.42
1	B	105	LYS	CB-CA-C	5.16	120.69	110.42
1	B	376	TRP	N-CA-C	5.09	116.03	108.86
1	B	101	ALA	CB-CA-C	-5.03	104.12	109.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4226	0	4131	78	0
1	B	4226	0	4131	109	0
2	A	9	0	5	1	0
2	B	9	0	5	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	8472	0	8272	185	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 11.

All (185) 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:105:LYS:HE2	1:B:106:ASN:H	1.07	1.11
1:B:40:ARG:HH11	1:B:40:ARG:HB2	1.02	1.07
1:B:105:LYS:HE2	1:B:106:ASN:N	1.74	1.02
1:B:105:LYS:CE	1:B:106:ASN:H	1.78	0.96
1:A:164:GLY:C	1:A:166:MET:HE2	1.95	0.90
1:B:40:ARG:HB2	1:B:40:ARG:NH1	1.88	0.89
1:A:370:LEU:O	1:A:374:THR:HB	1.73	0.88
1:A:164:GLY:CA	1:A:166:MET:HE2	2.06	0.85
1:B:370:LEU:O	1:B:374:THR:HB	1.79	0.82
1:B:164:GLY:CA	1:B:166:MET:HE2	2.09	0.82
1:B:164:GLY:C	1:B:166:MET:HE2	2.07	0.78
1:A:24:THR:O	1:A:101:ALA:HB2	1.83	0.78
1:B:302:MET:HB3	1:B:305:ILE:HD12	1.66	0.78
1:A:497:GLU:OE2	1:A:499:LYS:HE3	1.87	0.74
1:B:40:ARG:HH11	1:B:40:ARG:CB	1.91	0.73
1:A:449:PRO:HA	1:A:456:TYR:CD1	2.23	0.73
1:B:166:MET:HE3	1:B:166:MET:H	1.52	0.73
1:A:506:GLU:HG2	1:A:507:SER:H	1.53	0.73
1:B:449:PRO:HA	1:B:456:TYR:CD1	2.24	0.72
1:A:506:GLU:CG	1:A:507:SER:H	2.01	0.72
1:B:506:GLU:HG2	1:B:507:SER:H	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:HG22	1:A:377:VAL:O	1.90	0.71
1:B:506:GLU:CG	1:B:507:SER:H	2.03	0.70
1:B:319:VAL:O	1:B:418:PHE:HA	1.93	0.69
1:A:40:ARG:HB2	1:A:40:ARG:NH1	2.08	0.68
1:A:302:MET:HB2	1:A:305:ILE:HD12	1.76	0.68
1:B:13:VAL:HG12	1:B:56:TRP:HB3	1.76	0.67
1:A:166:MET:HE3	1:A:166:MET:H	1.60	0.65
1:B:40:ARG:HA	1:B:265:ARG:HH21	1.60	0.65
1:B:379:ASP:OD2	1:B:381:ARG:HG3	1.97	0.65
1:A:377:VAL:HG23	1:B:459:ALA:HB2	1.79	0.64
1:A:37:PRO:HD3	1:A:93:LEU:HD22	1.78	0.64
1:B:105:LYS:HB3	1:B:105:LYS:NZ	2.13	0.64
1:A:319:VAL:O	1:A:418:PHE:HA	1.98	0.63
1:A:42:ARG:O	1:A:43:PHE:HB2	1.98	0.63
1:A:97:VAL:HG12	1:A:99:ILE:CD1	2.29	0.63
1:B:482:GLU:O	1:B:486:ASN:HB3	1.99	0.63
1:B:321:VAL:HG21	1:B:399:ILE:HG12	1.81	0.62
1:A:482:GLU:O	1:A:486:ASN:HB3	2.00	0.62
1:B:125:LEU:HD12	1:B:128:TYR:CE2	2.36	0.60
1:B:37:PRO:HD3	1:B:93:LEU:HD22	1.82	0.60
1:A:102:PRO:O	1:A:103:LYS:C	2.44	0.60
1:A:379:ASP:OD2	1:A:381:ARG:HG3	2.02	0.59
1:B:164:GLY:HA2	1:B:166:MET:HE2	1.83	0.59
1:B:156:LEU:HD12	1:B:261:ILE:CD1	2.33	0.59
1:A:13:VAL:HG12	1:A:56:TRP:HB3	1.84	0.59
1:B:24:THR:O	1:B:101:ALA:CB	2.51	0.59
1:B:84:PRO:HG2	1:B:88:LEU:HD11	1.83	0.58
1:B:377:VAL:HG22	1:B:377:VAL:O	2.02	0.58
1:A:40:ARG:HA	1:A:265:ARG:HH21	1.68	0.58
1:A:105:LYS:NZ	1:A:106:ASN:H	2.02	0.58
1:B:221:ILE:C	1:B:222:LEU:HD12	2.29	0.58
1:A:486:ASN:C	1:A:486:ASN:OD1	2.47	0.57
1:A:98:TRP:C	1:A:99:ILE:HD12	2.30	0.57
1:B:97:VAL:HG12	1:B:99:ILE:CD1	2.35	0.57
1:A:105:LYS:HZ3	1:A:106:ASN:H	1.52	0.56
1:A:97:VAL:HG12	1:A:99:ILE:HD11	1.87	0.55
1:A:378:ASP:C	1:A:380:GLN:N	2.64	0.55
1:B:198:SER:OG	2:B:999:BEZ:H6	2.07	0.55
1:B:27:ALA:HB1	1:B:29:LEU:HD13	1.89	0.55
1:A:105:LYS:CE	1:A:106:ASN:H	2.20	0.55
1:B:24:THR:O	1:B:101:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:SER:O	1:B:508:THR:CG2	2.55	0.54
1:A:227:PHE:CD1	1:A:227:PHE:C	2.85	0.54
1:A:198:SER:OG	2:A:999:BEZ:H6	2.07	0.54
1:A:156:LEU:HD12	1:A:261:ILE:CD1	2.38	0.54
1:B:156:LEU:HD12	1:B:261:ILE:HD11	1.89	0.54
1:B:43:PHE:CE1	1:B:154:LEU:HD22	2.44	0.53
1:B:11:GLY:HA2	1:B:51:LYS:NZ	2.24	0.53
1:B:97:VAL:HG12	1:B:99:ILE:HD11	1.89	0.53
1:B:486:ASN:OD1	1:B:486:ASN:C	2.51	0.53
1:B:95:LEU:C	1:B:95:LEU:HD12	2.34	0.53
1:B:431:PRO:HD2	1:B:434:MET:SD	2.48	0.53
1:B:469:LYS:HG2	1:B:482:GLU:HG2	1.90	0.53
1:B:140:ILE:HG21	1:B:182:ILE:HD11	1.89	0.53
1:B:102:PRO:O	1:B:103:LYS:C	2.52	0.53
1:A:459:ALA:HB2	1:B:377:VAL:HG23	1.89	0.53
1:B:161:GLU:HB3	1:B:261:ILE:HG21	1.91	0.53
1:B:506:GLU:HG2	1:B:507:SER:N	2.23	0.53
1:A:164:GLY:HA2	1:A:166:MET:CE	2.39	0.52
1:A:140:ILE:HG21	1:A:182:ILE:HD11	1.90	0.52
1:A:469:LYS:HG2	1:A:482:GLU:HG2	1.92	0.52
1:A:164:GLY:HA2	1:A:166:MET:HE2	1.90	0.52
1:B:54:ASP:OD1	1:B:54:ASP:N	2.43	0.51
1:B:137:GLU:OE2	1:B:469:LYS:HE3	2.11	0.51
1:B:479:ASN:OD1	1:B:481:ASN:ND2	2.44	0.51
1:A:164:GLY:CA	1:A:166:MET:CE	2.84	0.51
1:B:378:ASP:C	1:B:380:GLN:N	2.68	0.51
1:A:156:LEU:HD12	1:A:261:ILE:HD11	1.92	0.50
1:A:506:GLU:HG2	1:A:507:SER:N	2.23	0.50
1:B:164:GLY:HA2	1:B:166:MET:CE	2.41	0.49
1:A:154:LEU:HD11	1:A:243:THR:HG23	1.94	0.49
1:A:105:LYS:HE2	1:A:106:ASN:OD1	2.13	0.49
1:B:206:LEU:HD22	1:B:299:LEU:HD11	1.94	0.49
1:B:95:LEU:HD12	1:B:95:LEU:O	2.13	0.49
1:B:361:VAL:O	1:B:366:LYS:HE3	2.13	0.48
1:B:166:MET:H	1:B:166:MET:CE	2.24	0.48
1:B:526:PHE:HB3	1:B:527:PRO:HD3	1.95	0.48
1:B:97:VAL:CG1	1:B:99:ILE:HD11	2.44	0.48
1:A:97:VAL:CG1	1:A:99:ILE:HD11	2.44	0.48
1:B:118:PHE:O	1:B:148:VAL:HB	2.14	0.48
1:B:227:PHE:C	1:B:227:PHE:CD1	2.91	0.48
1:B:502:THR:HG22	1:B:508:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:ASP:O	1:A:380:GLN:N	2.48	0.47
1:A:100:PRO:HG2	1:A:104:PRO:HG3	1.95	0.47
1:B:25:VAL:HG13	1:B:99:ILE:O	2.14	0.47
1:A:161:GLU:HB3	1:A:261:ILE:HG21	1.97	0.47
1:B:209:LEU:O	1:B:211:PRO:HD3	2.14	0.47
1:A:164:GLY:C	1:A:166:MET:CE	2.79	0.47
1:B:346:THR:O	1:B:347:ARG:C	2.58	0.47
1:B:414:ASN:ND2	1:B:414:ASN:H	2.13	0.47
1:B:99:ILE:HD12	1:B:99:ILE:N	2.30	0.47
1:B:362:SER:C	1:B:364:PHE:N	2.72	0.46
1:A:84:PRO:HG2	1:A:88:LEU:HD11	1.96	0.46
1:A:479:ASN:OD1	1:A:481:ASN:ND2	2.49	0.46
1:B:414:ASN:H	1:B:414:ASN:HD22	1.61	0.46
1:A:377:VAL:O	1:A:377:VAL:CG2	2.62	0.46
1:B:507:SER:O	1:B:508:THR:HG22	2.15	0.46
1:A:97:VAL:HG12	1:A:99:ILE:HD12	1.97	0.46
1:B:11:GLY:HA2	1:B:51:LYS:HZ1	1.78	0.46
1:B:152:GLY:O	1:B:166:MET:HE3	2.15	0.46
1:B:414:ASN:ND2	1:B:414:ASN:N	2.63	0.46
1:A:378:ASP:C	1:A:380:GLN:H	2.22	0.46
1:A:11:GLY:HA2	1:A:51:LYS:NZ	2.31	0.46
1:B:74:PRO:HA	1:B:80:GLU:OE2	2.16	0.46
1:A:27:ALA:HB1	1:A:29:LEU:HD13	1.98	0.45
1:A:110:LEU:HB3	1:A:195:PHE:CE2	2.52	0.45
1:A:137:GLU:OE2	1:A:469:LYS:HE2	2.15	0.45
1:A:362:SER:C	1:A:364:PHE:N	2.74	0.45
1:B:348:LYS:O	1:B:352:GLU:HG2	2.17	0.45
1:B:24:THR:O	1:B:101:ALA:HB3	2.15	0.45
1:B:506:GLU:CG	1:B:507:SER:N	2.77	0.45
1:B:198:SER:HB2	1:B:438:HIS:CE1	2.51	0.45
1:A:274:LEU:HD23	1:A:274:LEU:O	2.17	0.45
1:A:99:ILE:HD12	1:A:99:ILE:N	2.32	0.44
1:A:449:PRO:HA	1:A:456:TYR:HD1	1.80	0.44
1:B:54:ASP:HB2	1:B:55:ILE:H	1.59	0.44
1:B:18:LEU:CD1	1:B:27:ALA:HB2	2.48	0.44
1:B:40:ARG:HA	1:B:265:ARG:NH2	2.31	0.44
1:B:261:ILE:O	1:B:265:ARG:HB2	2.17	0.44
1:A:502:THR:HG22	1:A:508:THR:HA	2.00	0.44
1:B:156:LEU:HD13	1:B:257:GLU:HG2	1.99	0.44
1:B:461:GLU:O	1:B:465:ARG:HB2	2.18	0.44
1:B:502:THR:HB	1:B:509:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:O	1:A:200:GLY:N	2.47	0.43
1:A:40:ARG:HB2	1:A:40:ARG:HH11	1.80	0.43
1:B:310:GLY:HA2	1:B:312:PHE:CE2	2.54	0.43
1:B:464:SER:O	1:B:468:VAL:HG23	2.19	0.43
1:B:113:ILE:O	1:B:200:GLY:HA3	2.19	0.43
1:B:362:SER:C	1:B:364:PHE:H	2.26	0.43
1:B:105:LYS:NZ	1:B:106:ASN:H	2.16	0.43
1:B:125:LEU:HD12	1:B:128:TYR:CZ	2.53	0.43
1:B:201:ALA:HB1	1:B:225:GLY:O	2.19	0.43
1:A:40:ARG:O	1:A:40:ARG:HG3	2.16	0.43
1:B:274:LEU:HD23	1:B:274:LEU:O	2.19	0.43
1:A:320:GLY:HA3	1:A:419:TYR:CE2	2.54	0.43
1:A:308:GLU:O	1:A:308:GLU:HG3	2.17	0.42
1:B:378:ASP:O	1:B:379:ASP:OD2	2.37	0.42
1:B:99:ILE:HG13	1:B:140:ILE:HG12	2.01	0.42
1:B:156:LEU:HD12	1:B:261:ILE:HD13	2.00	0.42
1:B:519:CYS:O	1:B:523:THR:OG1	2.28	0.42
1:B:76:PHE:CE2	1:B:78:GLY:HA3	2.55	0.42
1:B:280:VAL:HG23	1:B:281:PRO:HD2	2.02	0.42
1:A:280:VAL:HG23	1:A:281:PRO:HD2	2.02	0.42
1:B:378:ASP:C	1:B:380:GLN:H	2.27	0.41
1:B:449:PRO:HA	1:B:456:TYR:HD1	1.78	0.41
1:A:524:SER:O	1:A:528:LYS:HG2	2.20	0.41
1:B:445:VAL:HG13	1:B:471:TRP:CD1	2.56	0.41
1:B:195:PHE:HD2	1:B:195:PHE:H	1.69	0.41
1:B:428:LEU:HA	1:B:429:PRO:HD3	1.79	0.41
1:A:506:GLU:CG	1:A:507:SER:N	2.75	0.41
1:B:42:ARG:O	1:B:43:PHE:HB2	2.20	0.41
1:A:40:ARG:HA	1:A:265:ARG:NH2	2.34	0.41
1:A:320:GLY:HA3	1:A:419:TYR:CZ	2.56	0.41
1:A:526:PHE:HB3	1:A:527:PRO:HD3	2.02	0.41
1:B:80:GLU:HG2	1:B:83:ASN:HD22	1.86	0.41
1:A:40:ARG:HB2	1:A:40:ARG:CZ	2.50	0.41
1:A:167:GLY:O	1:A:170:ASP:HB2	2.21	0.41
1:A:195:PHE:HB3	1:A:221:ILE:HB	2.01	0.41
1:A:221:ILE:C	1:A:222:LEU:HD12	2.46	0.40
1:B:195:PHE:HB3	1:B:221:ILE:HB	2.04	0.40
1:A:42:ARG:O	1:A:43:PHE:CB	2.69	0.40
1:B:200:GLY:O	1:B:204:VAL:HG23	2.20	0.40
1:A:428:LEU:HA	1:A:429:PRO:HD3	1.83	0.40
1:B:97:VAL:HG12	1:B:99:ILE:HD12	2.03	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	529/574 (92%)	477 (90%)	46 (9%)	6 (1%)	11	40
1	B	529/574 (92%)	477 (90%)	46 (9%)	6 (1%)	11	40
All	All	1058/1148 (92%)	954 (90%)	92 (9%)	12 (1%)	11	40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	B	379	ASP
1	A	347	ARG
1	A	488	THR
1	B	105	LYS
1	B	363	GLU
1	B	488	THR
1	B	506	GLU
1	B	513	LYS
1	A	198	SER
1	A	506	GLU
1	A	513	LYS

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	455/494 (92%)	416 (91%)	39 (9%)	10	34
1	B	455/494 (92%)	415 (91%)	40 (9%)	9	33
All	All	910/988 (92%)	831 (91%)	79 (9%)	9	33

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	35	GLN
1	A	40	ARG
1	A	55	ILE
1	A	65	CYS
1	A	71	GLN
1	A	92	CYS
1	A	93	LEU
1	A	103	LYS
1	A	105	LYS
1	A	108	THR
1	A	166	MET
1	A	195	PHE
1	A	252	CYS
1	A	253	SER
1	A	262	LYS
1	A	265	ARG
1	A	266	ASN
1	A	284	THR
1	A	308	GLU
1	A	338	SER
1	A	363	GLU
1	A	364	PHE
1	A	367	GLU
1	A	368	SER
1	A	374	THR
1	A	377	VAL
1	A	381	ARG
1	A	383	GLU
1	A	411	GLU
1	A	428	LEU
1	A	465	ARG
1	A	486	ASN
1	A	487	SER
1	A	495	SER

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Mol	Chain	Res	Type
1	A	497	GLU
1	A	502	THR
1	A	528	LYS
1	A	533	THR
1	B	4	ILE
1	B	19	THR
1	B	29	LEU
1	B	40	ARG
1	B	55	ILE
1	B	92	CYS
1	B	93	LEU
1	B	105	LYS
1	B	108	THR
1	B	166	MET
1	B	176	GLN
1	B	195	PHE
1	B	252	CYS
1	B	253	SER
1	B	262	LYS
1	B	265	ARG
1	B	274	LEU
1	B	284	THR
1	B	302	MET
1	B	338	SER
1	B	363	GLU
1	B	368	SER
1	B	374	THR
1	B	377	VAL
1	B	383	GLU
1	B	410	SER
1	B	411	GLU
1	B	414	ASN
1	B	427	LYS
1	B	428	LEU
1	B	452	ARG
1	B	465	ARG
1	B	469	LYS
1	B	486	ASN
1	B	487	SER
1	B	495	SER
1	B	496	THR
1	B	497	GLU

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Mol	Chain	Res	Type
1	B	502	THR
1	B	533	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	172	GLN
1	A	181	ASN
1	A	223	GLN
1	A	351	GLN
1	B	35	GLN
1	B	266	ASN
1	B	351	GLN
1	B	517	GLN

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](#)

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	BEZ	A	999	-	9,9,9	0.79	0	11,11,11	0.79	0
2	BEZ	B	999	-	9,9,9	1.07	0	11,11,11	1.05	1 (9%)

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	BEZ	A	999	-	-	1/4/4/4	0/1/1/1
2	BEZ	B	999	-	-	4/4/4/4	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	999	BEZ	O2-C-O1	-2.68	117.59	123.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	999	BEZ	O2-C-C1-C2
2	B	999	BEZ	O2-C-C1-C6
2	B	999	BEZ	O1-C-C1-C2
2	B	999	BEZ	O1-C-C1-C6
2	A	999	BEZ	O2-C-C1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	BEZ	1	0
2	B	999	BEZ	1	0

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

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	531/574 (92%)	0.01	14 (2%) 57 38	34, 53, 79, 95	0
1	B	531/574 (92%)	-0.01	10 (1%) 66 47	34, 53, 79, 94	0
All	All	1062/1148 (92%)	0.00	24 (2%) 61 42	34, 53, 79, 95	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ASP	4.9
1	B	377	VAL	3.7
1	B	105	LYS	3.5
1	A	364	PHE	3.5
1	B	75	GLY	3.4
1	B	364	PHE	3.2
1	A	488	THR	3.2
1	A	377	VAL	3.1
1	A	105	LYS	3.0
1	B	379	ASP	2.8
1	B	488	THR	2.7
1	A	378	ASP	2.6
1	A	380	GLN	2.6
1	A	484	GLN	2.6
1	A	274	LEU	2.6
1	A	256	ASN	2.5
1	B	378	ASP	2.3
1	A	533	THR	2.3
1	A	87	ASP	2.2
1	B	485	ASN	2.1
1	B	50	THR	2.1
1	A	534	GLY	2.1
1	B	484	GLN	2.0
1	A	282	TYR	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	BEZ	B	999	9/9	0.91	0.17	71,73,75,75	0
2	BEZ	A	999	9/9	0.94	0.16	70,73,75,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.