



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 3WYN / pdb_00003wyn
Title : Structure of calcium bound cutinase Est119 from *Thermobifida alba*.
Authors : Kitadokoro, K.; Thumarat, U.; Kawai, F.
Deposited on : 2014-09-02
Resolution : 1.68 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

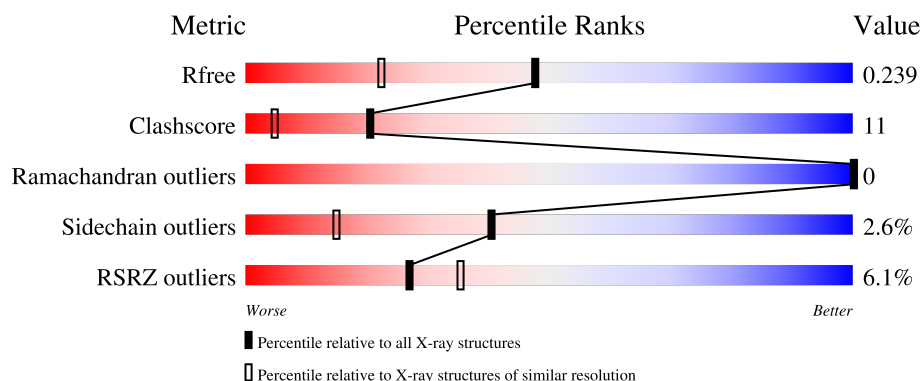
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	306	
1	B	306	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4464 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 Esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2003	1256	351	389	7			
1	B	261	Total	C	N	O	S	0	0	0
			2009	1262	351	389	7			

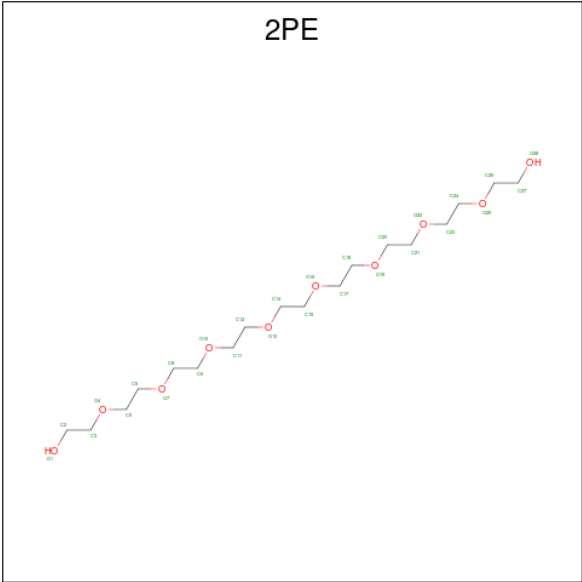
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP F7IX06
A	-4	HIS	-	expression tag	UNP F7IX06
A	-3	HIS	-	expression tag	UNP F7IX06
A	-2	HIS	-	expression tag	UNP F7IX06
A	-1	HIS	-	expression tag	UNP F7IX06
A	0	HIS	-	expression tag	UNP F7IX06
B	-5	HIS	-	expression tag	UNP F7IX06
B	-4	HIS	-	expression tag	UNP F7IX06
B	-3	HIS	-	expression tag	UNP F7IX06
B	-2	HIS	-	expression tag	UNP F7IX06
B	-1	HIS	-	expression tag	UNP F7IX06
B	0	HIS	-	expression tag	UNP F7IX06

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			24	16	8		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	214	Total	O	0	0
			214	214		
4	B	211	Total	O	0	0
			211	211		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.47Å 87.74Å 72.62Å 90.00° 133.35° 90.00°	Depositor
Resolution (Å)	31.26 – 1.68 31.26 – 1.68	Depositor EDS
% Data completeness (in resolution range)	97.8 (31.26-1.68) 97.8 (31.26-1.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.237 0.197 , 0.239	Depositor DCC
R_{free} test set	2613 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h+2*k,-h-l 0.000 for h,-k,-h-l 0.028 for -h-2*k,-k,l	Xtriage
F_o , F_c correlation	0.96	EDS
Total number of atoms	4464	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 2PE

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	1.78	40/2053 (1.9%)	1.78	48/2796 (1.7%)
1	B	1.37	10/2060 (0.5%)	1.38	18/2807 (0.6%)
All	All	1.59	50/4113 (1.2%)	1.59	66/5603 (1.2%)

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	1
1	B	0	1
All	All	0	2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	ILE	N-CA	11.76	1.55	1.46
1	A	175	THR	C-O	10.38	1.36	1.24
1	A	263	ALA	C-O	9.74	1.35	1.24
1	B	190	PRO	C-O	-9.69	1.14	1.23
1	A	259	MET	C-O	9.67	1.35	1.24
1	B	170	MET	N-CA	8.50	1.56	1.46
1	A	209	ILE	C-O	-8.29	1.15	1.24
1	A	173	GLY	C-O	8.28	1.33	1.23
1	A	181	GLN	N-CA	7.96	1.56	1.46
1	A	265	LEU	N-CA	7.70	1.55	1.46
1	A	257	ILE	N-CA	7.44	1.55	1.46
1	A	117	GLY	N-CA	7.37	1.56	1.45
1	A	261	SER	C-O	7.21	1.32	1.24
1	A	174	GLY	N-CA	7.14	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	LYS	C-O	7.11	1.31	1.24
1	A	268	PHE	N-CA	6.58	1.54	1.46
1	A	263	ALA	N-CA	6.51	1.54	1.46
1	B	261	SER	N-CA	6.49	1.54	1.46
1	A	203	ILE	CA-CB	6.41	1.61	1.53
1	A	227	PHE	N-CA	6.20	1.53	1.46
1	A	110	GLY	N-CA	6.08	1.53	1.45
1	A	90	TYR	C-O	6.04	1.31	1.23
1	A	177	ARG	N-CA	6.01	1.53	1.46
1	A	267	ARG	C-O	5.98	1.31	1.24
1	A	275	TYR	N-CA	5.70	1.53	1.46
1	A	120	VAL	CA-CB	5.69	1.61	1.54
1	A	176	LEU	C-O	5.56	1.30	1.24
1	A	262	VAL	C-O	5.52	1.30	1.24
1	A	185	LEU	C-O	5.50	1.31	1.23
1	A	139	LEU	CA-C	5.41	1.59	1.52
1	B	218	ALA	N-CA	5.38	1.54	1.46
1	A	124	ASP	C-O	5.38	1.30	1.23
1	A	264	TRP	C-O	5.37	1.30	1.24
1	B	219	SER	C-O	5.37	1.30	1.23
1	A	266	LYS	C-O	5.37	1.30	1.24
1	B	107	ALA	C-O	-5.36	1.17	1.24
1	B	175	THR	CA-C	5.29	1.59	1.52
1	A	58	SER	CA-C	-5.27	1.46	1.52
1	A	187	ALA	CA-CB	-5.26	1.44	1.53
1	B	159	ASP	N-CA	5.25	1.53	1.46
1	A	258	GLY	C-O	5.19	1.29	1.23
1	A	100	THR	CA-CB	5.18	1.61	1.53
1	A	174	GLY	C-O	5.17	1.29	1.23
1	A	204	THR	C-N	5.13	1.39	1.33
1	A	168	HIS	N-CA	5.12	1.52	1.46
1	B	122	ALA	CA-CB	5.12	1.60	1.53
1	B	122	ALA	N-CA	-5.10	1.40	1.46
1	A	220	VAL	N-CA	5.06	1.52	1.46
1	A	97	PRO	N-CA	5.05	1.52	1.47
1	A	205	VAL	CA-C	5.02	1.58	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	ILE	N-CA-C	-9.14	94.97	108.12
1	A	112	ARG	NE-CZ-NH1	-8.96	112.53	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	LEU	N-CA-C	-8.81	101.76	111.36
1	A	171	GLY	CA-C-N	8.68	129.40	119.94
1	A	171	GLY	C-N-CA	8.68	129.40	119.94
1	B	217	ILE	N-CA-C	-8.61	104.92	111.90
1	A	142	ALA	N-CA-C	8.52	120.56	111.28
1	A	233	SER	N-CA-C	-7.70	99.45	110.08
1	A	211	GLY	N-CA-C	-7.45	99.72	111.18
1	A	96	SER	CB-CA-C	-7.37	98.43	108.68
1	A	205	VAL	O-C-N	7.30	129.42	121.10
1	A	246	SER	O-C-N	7.29	131.62	122.43
1	A	209	ILE	CA-C-N	-7.19	113.82	123.10
1	A	209	ILE	C-N-CA	-7.19	113.82	123.10
1	A	242	LEU	N-CA-C	-7.15	98.40	109.76
1	A	246	SER	N-CA-C	-6.78	99.94	110.17
1	A	123	ILE	N-CA-C	6.72	118.80	109.45
1	A	93	ILE	CB-CA-C	-6.67	100.59	110.33
1	A	236	ASP	CA-C-N	-6.51	109.98	122.09
1	A	236	ASP	C-N-CA	-6.51	109.98	122.09
1	A	206	PRO	N-CA-C	-6.45	101.10	111.03
1	A	205	VAL	CA-C-O	-6.28	111.53	119.95
1	A	176	LEU	N-CA-C	-6.26	104.38	111.07
1	B	171	GLY	CA-C-N	6.23	126.85	120.00
1	B	171	GLY	C-N-CA	6.23	126.85	120.00
1	A	173	GLY	N-CA-C	-6.18	105.33	112.50
1	B	59	GLY	CA-C-N	6.15	127.05	120.47
1	B	59	GLY	C-N-CA	6.15	127.05	120.47
1	B	172	GLY	N-CA-C	-6.04	105.04	112.77
1	A	109	LEU	N-CA-C	-5.88	104.46	111.69
1	A	213	GLU	N-CA-C	-5.85	104.91	111.28
1	A	215	ASP	N-CA-CB	-5.84	101.14	109.85
1	B	200	TRP	N-CA-C	-5.78	103.50	110.44
1	A	246	SER	CA-C-O	-5.76	114.39	121.88
1	A	235	THR	CA-C-O	-5.61	114.88	121.16
1	B	193	PRO	N-CA-C	5.55	119.73	111.41
1	A	207	THR	O-C-N	5.51	129.76	123.31
1	B	123	ILE	N-CA-C	5.48	117.60	109.17
1	B	112	ARG	N-CA-C	-5.47	105.40	111.36
1	A	256	THR	N-CA-C	-5.44	104.76	111.40
1	A	239	TYR	N-CA-C	-5.41	99.28	108.26
1	A	56	ALA	N-CA-C	5.38	117.48	110.43
1	A	182	ARG	CA-C-N	5.38	126.56	119.84
1	A	182	ARG	C-N-CA	5.38	126.56	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	LEU	N-CA-C	-5.32	105.38	111.07
1	A	274	ARG	N-CA-C	-5.32	106.63	113.01
1	A	205	VAL	CA-C-N	5.31	125.56	119.83
1	A	205	VAL	C-N-CA	5.31	125.56	119.83
1	B	152	SER	N-CA-C	5.27	117.71	111.33
1	B	209	ILE	CA-C-N	-5.26	116.28	123.12
1	B	209	ILE	C-N-CA	-5.26	116.28	123.12
1	B	231	ILE	CB-CA-C	5.25	116.72	110.68
1	B	41	ASN	CA-C-N	5.24	125.55	119.47
1	B	41	ASN	C-N-CA	5.24	125.55	119.47
1	A	161	SER	CA-C-N	-5.18	114.32	122.76
1	A	161	SER	C-N-CA	-5.18	114.32	122.76
1	A	120	VAL	CB-CA-C	-5.17	102.78	110.33
1	A	237	LYS	N-CA-C	-5.16	100.30	108.14
1	A	230	SER	CA-C-N	-5.14	118.89	122.59
1	A	230	SER	C-N-CA	-5.14	118.89	122.59
1	A	113	ILE	CA-C-N	5.12	127.39	120.38
1	A	113	ILE	C-N-CA	5.12	127.39	120.38
1	B	193	PRO	CB-CA-C	-5.12	104.25	110.95
1	A	59	GLY	CA-C-N	5.05	124.74	119.64
1	A	59	GLY	C-N-CA	5.05	124.74	119.64
1	A	114	ALA	O-C-N	-5.05	116.77	122.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	210	ILE	Mainchain
1	B	288	LEU	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	2003	0	1930	42	0
1	B	2009	0	1943	47	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	B	24	0	31	3	0
4	A	214	0	0	15	0
4	B	211	0	0	19	0
All	All	4464	0	3904	89	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 (89) 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:108:TRP:CZ2	4:A:675:HOH:O	1.96	1.15
1:A:38:GLN:N	1:A:38:GLN:OE1	1.88	1.05
1:B:252:ILE:O	4:B:672:HOH:O	1.76	1.02
1:B:284:ARG:HG2	1:B:288:LEU:HD21	1.40	1.02
1:B:248:PHE:HD2	4:B:682:HOH:O	1.45	0.99
1:A:108:TRP:CH2	4:A:675:HOH:O	2.14	0.98
1:A:300:PHE:C	4:A:659:HOH:O	2.07	0.96
1:B:108:TRP:CZ2	4:B:672:HOH:O	2.19	0.96
1:B:252:ILE:C	4:B:672:HOH:O	2.06	0.94
1:B:108:TRP:CE2	4:B:672:HOH:O	2.23	0.89
1:A:126:ASN:H	1:A:138:GLN:HE22	1.15	0.88
1:B:300:PHE:O	4:B:686:HOH:O	1.92	0.87
1:B:284:ARG:HG3	1:B:286:GLY:H	1.40	0.86
1:B:280:CYS:SG	4:B:568:HOH:O	2.36	0.81
1:A:38:GLN:N	1:A:38:GLN:CD	2.35	0.79
1:A:108:TRP:CE2	4:A:675:HOH:O	2.28	0.76
1:A:126:ASN:H	1:A:138:GLN:NE2	1.83	0.75
1:A:253:THR:HA	4:A:675:HOH:O	1.90	0.71
1:A:53:MET:HB3	4:A:700:HOH:O	1.90	0.70
1:A:116:HIS:HD2	4:A:570:HOH:O	1.75	0.69
1:A:126:ASN:N	1:A:138:GLN:HE22	1.89	0.69
1:B:253:THR:CA	4:B:672:HOH:O	2.42	0.67
1:B:116:HIS:HD2	4:B:608:HOH:O	1.80	0.64
1:A:237:LYS:HE2	4:A:563:HOH:O	1.97	0.63
1:B:253:THR:HA	4:B:672:HOH:O	1.96	0.63
1:B:284:ARG:CG	1:B:288:LEU:HD21	2.24	0.61
1:B:93:ILE:HD12	1:B:164:ALA:HB3	1.83	0.61
1:B:70:ARG:NH2	4:B:677:HOH:O	2.33	0.60
1:B:253:THR:N	4:B:672:HOH:O	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:H	1:B:287:LEU:CD2	2.15	0.60
1:B:298:CYS:HA	4:B:568:HOH:O	2.01	0.60
1:A:169:SER:HA	1:A:192:THR:O	2.03	0.59
1:B:284:ARG:HG2	1:B:288:LEU:CD2	2.26	0.59
1:B:281:PRO:HD2	4:B:590:HOH:O	2.02	0.58
1:A:253:THR:CA	4:A:675:HOH:O	2.48	0.57
1:B:288:LEU:HD23	1:B:288:LEU:H	1.71	0.56
1:B:131:GLN:HE22	3:B:401:2PE:H31	1.71	0.56
1:B:223:HIS:HE1	4:B:597:HOH:O	1.89	0.56
1:A:112:ARG:HD2	4:A:571:HOH:O	2.06	0.55
1:A:195:HIS:H	1:A:223:HIS:HD2	1.57	0.52
1:B:110:GLY:HA2	1:B:120:VAL:HG11	1.91	0.52
1:B:287:LEU:HD23	1:B:288:LEU:HD23	1.91	0.51
1:B:282:GLY:HA3	1:B:294:TYR:CE2	2.44	0.51
1:A:284:ARG:HG3	1:A:285:THR:N	2.26	0.51
1:A:199:SER:OG	1:A:201:ARG:HG3	2.11	0.51
1:B:236:ASP:OD1	1:B:300:PHE:HD1	1.95	0.50
1:B:170:MET:HE3	3:B:401:2PE:H81	1.93	0.50
1:A:191:LEU:O	1:A:192:THR:C	2.55	0.49
1:A:165:VAL:HG11	1:A:178:LEU:HD23	1.94	0.48
1:A:252:ILE:O	1:A:253:THR:C	2.53	0.48
1:A:44:GLU:HG3	4:A:667:HOH:O	2.13	0.48
1:A:44:GLU:OE2	4:A:667:HOH:O	2.20	0.48
1:B:168:HIS:CE1	1:B:192:THR:OG1	2.66	0.47
1:A:192:THR:N	1:A:193:PRO:HD3	2.30	0.47
1:A:192:THR:N	1:A:193:PRO:CD	2.78	0.47
1:A:166:MET:HG2	1:A:189:ILE:HB	1.96	0.47
1:B:192:THR:N	1:B:193:PRO:CD	2.78	0.46
1:B:70:ARG:HG2	4:B:631:HOH:O	2.16	0.46
1:B:169:SER:HA	1:B:192:THR:O	2.15	0.45
1:B:41:ASN:HA	1:B:42:PRO:HD2	1.82	0.45
1:A:252:ILE:O	4:A:675:HOH:O	2.21	0.45
1:A:254:ASN:N	4:A:675:HOH:O	2.49	0.45
1:A:116:HIS:HE1	4:A:547:HOH:O	2.01	0.44
1:B:284:ARG:HB2	4:B:630:HOH:O	2.16	0.44
1:B:297:THR:HG21	4:B:581:HOH:O	2.17	0.44
1:B:287:LEU:CD2	1:B:287:LEU:N	2.79	0.44
1:A:100:THR:HA	1:A:128:THR:HB	2.00	0.43
1:A:131:GLN:HB3	1:A:132:PRO:CD	2.48	0.43
1:A:249:ALA:N	1:A:250:PRO:CD	2.81	0.43
1:A:200:TRP:HB3	1:A:203:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:HIS:HE1	1:A:247:HIS:O	2.02	0.43
1:B:287:LEU:H	1:B:287:LEU:HD22	1.83	0.43
1:B:73:ALA:O	4:B:618:HOH:O	2.21	0.42
1:B:243:ASP:HA	1:B:292:GLU:HB2	2.01	0.42
1:A:195:HIS:H	1:A:223:HIS:CD2	2.36	0.42
1:A:87:ASN:HD22	1:A:157:ARG:NH2	2.18	0.42
1:B:112:ARG:HH11	1:B:112:ARG:HD2	1.76	0.42
1:A:236:ASP:OD1	1:A:300:PHE:HA	2.20	0.41
1:B:131:GLN:HE22	3:B:401:2PE:C3	2.33	0.41
1:A:75:GLY:O	1:A:138:GLN:HG2	2.20	0.41
1:A:165:VAL:HG23	1:A:175:THR:HG23	2.02	0.41
1:B:100:THR:HA	1:B:128:THR:HB	2.02	0.41
1:B:212:ALA:HB3	1:B:215:ASP:HB2	2.02	0.41
1:B:284:ARG:HG2	1:B:288:LEU:HD11	2.02	0.41
1:B:168:HIS:CD2	1:B:251:ASN:HD21	2.38	0.41
1:B:242:LEU:HB2	1:B:245:ALA:HB3	2.03	0.41
1:A:251:ASN:C	1:A:252:ILE:HG13	2.45	0.40
1:B:282:GLY:HA3	1:B:294:TYR:CD2	2.57	0.40
1:A:261:SER:O	1:A:265:LEU:HG	2.21	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	256/306 (84%)	247 (96%)	9 (4%)	0	100	100
1	B	259/306 (85%)	250 (96%)	9 (4%)	0	100	100
All	All	515/612 (84%)	497 (96%)	18 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	213/246 (87%)	206 (97%)	7 (3%)	33	8
1	B	214/246 (87%)	210 (98%)	4 (2%)	50	25
All	All	427/492 (87%)	416 (97%)	11 (3%)	40	15

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	57	ARG
1	A	109	LEU
1	A	132	PRO
1	A	206	PRO
1	A	209	ILE
1	A	284	ARG
1	B	70	ARG
1	B	233	SER
1	B	287	LEU
1	B	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	87	ASN
1	A	116	HIS
1	A	138	GLN
1	A	168	HIS
1	A	223	HIS
1	A	277	GLN
1	B	48	ASN
1	B	116	HIS
1	B	131	GLN
1	B	168	HIS

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Mol	Chain	Res	Type
1	B	223	HIS

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, 3 are 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	2PE	B	401	-	23,23,27	0.57	0	22,22,26	0.41	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
3	2PE	B	401	-	-	16/21/21/25	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

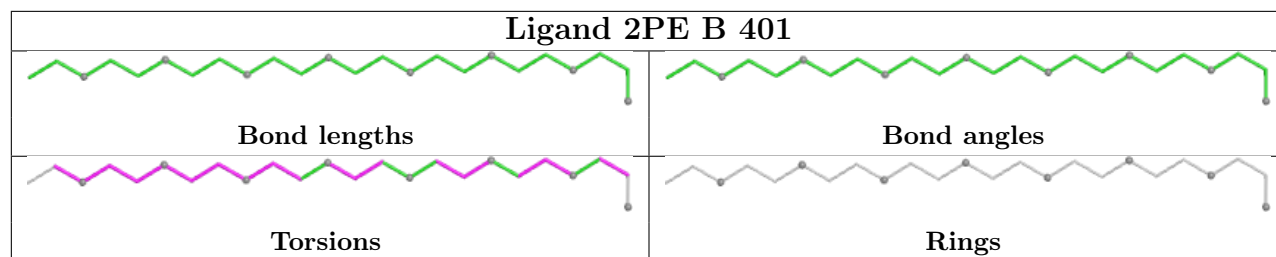
Mol	Chain	Res	Type	Atoms
3	B	401	2PE	O19-C20-C21-O22
3	B	401	2PE	O10-C11-C12-O13
3	B	401	2PE	O1-C2-C3-O4
3	B	401	2PE	O13-C14-C15-O16
3	B	401	2PE	C24-C23-O22-C21
3	B	401	2PE	C18-C17-O16-C15
3	B	401	2PE	C14-C15-O16-C17
3	B	401	2PE	C21-C20-O19-C18
3	B	401	2PE	C9-C8-O7-C6
3	B	401	2PE	C20-C21-O22-C23
3	B	401	2PE	C6-C5-O4-C3
3	B	401	2PE	O7-C8-C9-O10
3	B	401	2PE	O4-C5-C6-O7
3	B	401	2PE	C11-C12-O13-C14
3	B	401	2PE	O16-C17-C18-O19
3	B	401	2PE	C17-C18-O19-C20

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	2PE	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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	260/306 (84%)	0.59	7 (2%) 56 63	9, 19, 30, 51	0
1	B	261/306 (85%)	0.87	25 (9%) 13 16	14, 23, 41, 70	0
All	All	521/612 (85%)	0.73	32 (6%) 27 35	9, 20, 38, 70	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	LEU	5.7
1	B	106	ILE	5.4
1	B	288	LEU	4.8
1	B	300	PHE	4.2
1	A	289	SER	4.1
1	B	40	ALA	3.9
1	B	295	ARG	3.8
1	B	71	PHE	3.0
1	B	282	GLY	2.9
1	A	285	THR	2.9
1	A	87	ASN	2.9
1	B	285	THR	2.8
1	B	298	CYS	2.8
1	A	192	THR	2.8
1	B	281	PRO	2.7
1	B	70	ARG	2.7
1	B	291	VAL	2.7
1	B	294	TYR	2.7
1	B	214	TYR	2.6
1	B	278	PHE	2.5
1	B	284	ARG	2.3
1	B	192	THR	2.2
1	A	218	ALA	2.2
1	B	296	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASP	2.1
1	A	137	ARG	2.0
1	B	137	ARG	2.0
1	B	180	SER	2.0
1	B	87	ASN	2.0
1	B	286	GLY	2.0
1	B	252	ILE	2.0
1	B	233	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](#)

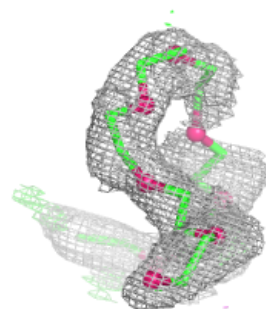
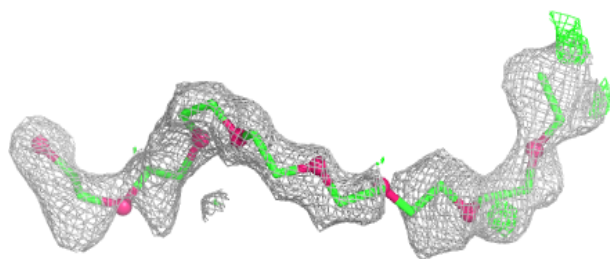
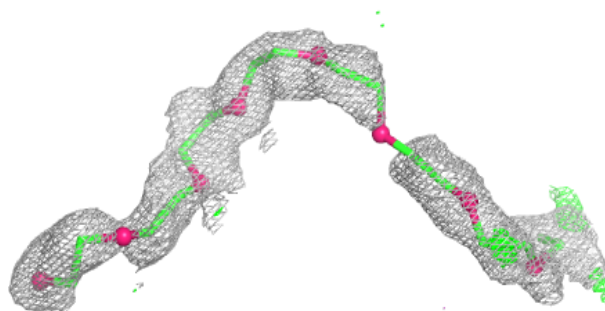
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	2PE	B	401	24/28	0.78	0.18	44,55,64,66	0
2	CA	B	402	1/1	0.90	0.12	53,53,53,53	0
2	CA	B	403	1/1	0.93	0.12	51,51,51,51	0
2	CA	A	401	1/1	0.94	0.15	37,37,37,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 2PE B 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.