



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:23 PM UTC

PDB ID : 1PSA / pdb_00001psa
Title : STRUCTURE OF A PEPSIN(SLASH)RENIN INHIBITOR COMPLEX REVEALS A NOVEL CRYSTAL PACKING INDUCED BY MINOR CHEMICAL ALTERATIONS IN THE INHIBITOR
Authors : Chen, L.; Abad-Zapatero, C.
Deposited on : 1991-10-22
Resolution : 2.90 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

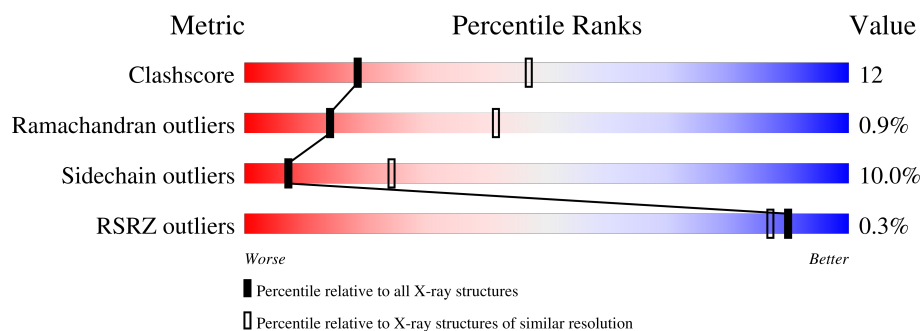
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	326	
1	B	326	

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	0ZL	A	327	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5044 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.

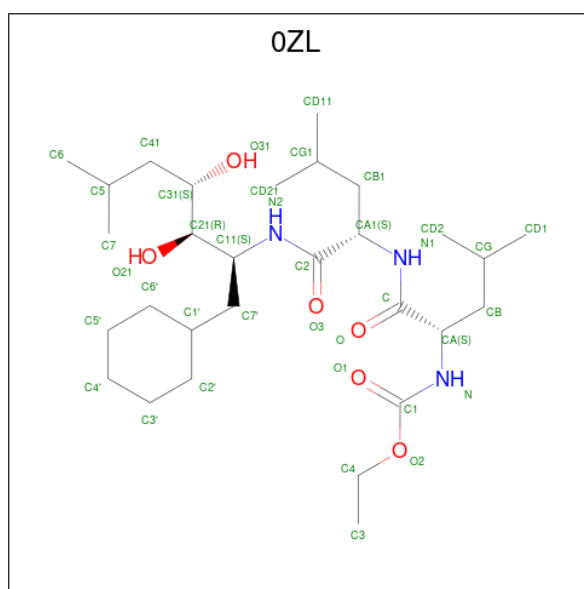
- Molecule 1 is a protein called PEPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	3	0	0
			2429	1530	366	523	10			
1	B	326	Total	C	N	O	S	3	0	0
			2429	1530	366	523	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP P00791
B	?	-	ILE	deletion	UNP P00791

- Molecule 2 is N-(ethoxycarbonyl)-L-leucyl-N-[(1R,2S,3S)-1-(cyclohexylmethyl)-2,3-dihydroxy-5-methylhexyl]-L-leucinamide (CCD ID: 0ZL) (formula: C₂₉H₅₅N₃O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	29	3	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			38	29	3	6		

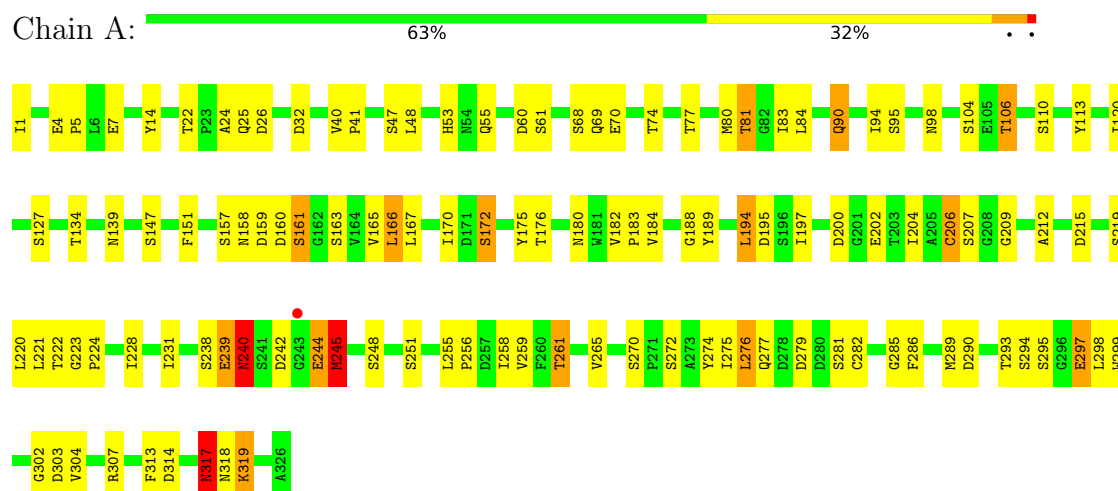
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total	O	0	0
			54	54		
3	B	56	Total	O	0	0
			56	56		

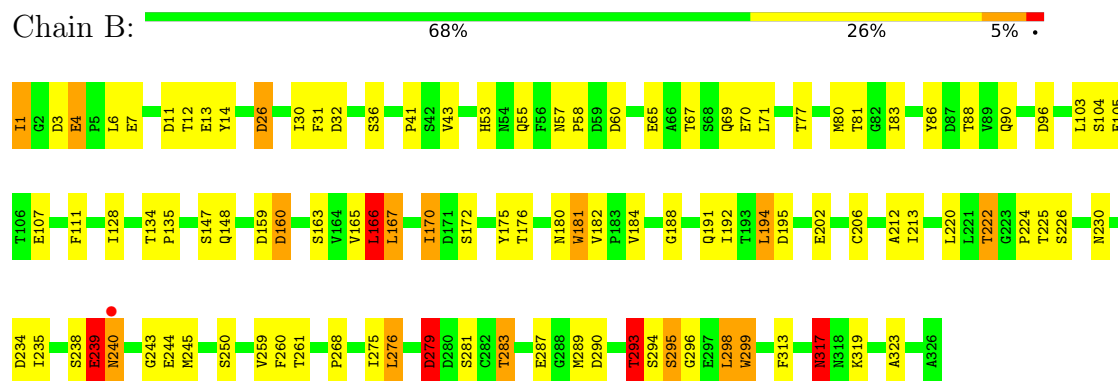
3 Residue-property plots

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: PEPSIN A



• Molecule 1: PEPSIN A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α , β , γ	54.10Å 74.40Å 76.50Å 90.00° 90.00° 100.80°	Depositor
Resolution (Å)	8.00 – 2.90 8.00 – 2.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.90) 90.5 (8.00-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.139 , (Not available) 0.129 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5044	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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: 0ZL

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	0.98	5/2484 (0.2%)	1.86	59/3400 (1.7%)
1	B	1.02	4/2484 (0.2%)	1.82	52/3400 (1.5%)
All	All	1.00	9/4968 (0.2%)	1.84	111/6800 (1.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	LEU	CB-CG	-9.62	1.34	1.53
1	B	166	LEU	CG-CD1	8.41	1.80	1.52
1	A	53	HIS	CD2-NE2	-6.81	1.30	1.37
1	B	53	HIS	CD2-NE2	-6.54	1.30	1.37
1	B	170	ILE	CA-CB	6.38	1.64	1.54
1	A	166	LEU	CG-CD1	5.79	1.71	1.52
1	A	166	LEU	CB-CG	-5.41	1.42	1.53
1	A	165	VAL	C-N	-5.29	1.24	1.33
1	A	170	ILE	CA-CB	5.05	1.61	1.54

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	ASP	CA-CB-CG	14.04	126.64	112.60
1	A	279	ASP	CA-CB-CG	13.32	125.92	112.60
1	A	26	ASP	CA-CB-CG	12.04	124.64	112.60
1	A	26	ASP	CB-CA-C	-10.10	92.47	109.53
1	A	317	ASN	OD1-CG-ND2	-8.61	114.00	122.60
1	A	26	ASP	N-CA-CB	8.43	122.78	110.06
1	B	298	LEU	N-CA-C	8.08	121.89	110.50
1	A	159	ASP	CA-CB-CG	7.91	120.50	112.60
1	B	240	ASN	CA-CB-CG	7.81	120.41	112.60
1	B	26	ASP	CA-CB-CG	7.67	120.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ASP	CA-CB-CG	7.67	120.27	112.60
1	A	161	SER	O-C-N	-7.63	113.68	122.68
1	A	184	VAL	O-C-N	-7.36	115.16	122.67
1	A	139	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	317	ASN	CB-CG-ND2	7.23	127.25	116.40
1	B	317	ASN	OD1-CG-ND2	-7.17	115.43	122.60
1	A	215	ASP	CA-CB-CG	7.01	119.61	112.60
1	A	314	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	11	ASP	CA-CB-CG	6.74	119.34	112.60
1	B	159	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	160	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	181	TRP	CG-CD2-CE3	6.62	140.52	133.90
1	A	239	GLU	CB-CG-CD	6.60	123.83	112.60
1	A	160	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	60	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	40	VAL	O-C-N	-6.41	117.24	121.72
1	A	240	ASN	CA-CB-CG	6.38	118.98	112.60
1	B	184	VAL	N-CA-C	-6.38	100.42	108.84
1	B	107	GLU	CA-C-N	6.33	126.28	119.76
1	B	107	GLU	C-N-CA	6.33	126.28	119.76
1	A	53	HIS	CB-CG-CD2	-6.33	122.97	131.20
1	A	318	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	90	GLN	CG-CD-NE2	6.22	125.73	116.40
1	B	165	VAL	N-CA-C	-6.20	98.70	107.75
1	A	244	GLU	N-CA-C	-6.18	103.29	111.02
1	A	81	THR	N-CA-C	-6.18	99.74	109.50
1	B	293	THR	CA-CB-OG1	-6.18	100.33	109.60
1	A	60	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	200	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	323	ALA	O-C-N	-6.10	117.07	121.83
1	B	293	THR	N-CA-CB	-6.10	101.73	111.43
1	B	105	GLU	N-CA-C	-6.04	105.81	113.43
1	B	12	THR	CA-CB-OG1	-6.02	100.57	109.60
1	A	270	SER	CA-C-N	6.00	126.17	119.32
1	A	270	SER	C-N-CA	6.00	126.17	119.32
1	B	181	TRP	CB-CG-CD1	-6.00	117.89	126.90
1	A	258	ILE	N-CA-C	-6.00	99.75	108.87
1	A	158	ASN	N-CA-C	5.93	119.82	112.58
1	A	206	CYS	N-CA-CB	-5.90	101.08	111.40
1	B	81	THR	N-CA-C	-5.87	100.33	109.72
1	B	230	ASN	CA-CB-CG	-5.85	106.75	112.60
1	A	240	ASN	N-CA-CB	-5.80	100.68	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	MET	N-CA-C	-5.79	97.08	107.98
1	A	24	ALA	N-CA-C	5.79	118.96	109.76
1	A	70	GLU	CB-CG-CD	5.78	122.43	112.60
1	A	7	GLU	CB-CG-CD	5.78	122.42	112.60
1	A	290	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	317	ASN	CA-CB-CG	5.76	118.36	112.60
1	B	70	GLU	O-C-N	-5.74	116.04	122.75
1	B	170	ILE	O-C-N	-5.74	116.95	122.97
1	A	180	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	A	319	LYS	CB-CG-CD	-5.64	98.32	111.30
1	A	313	PHE	N-CA-C	-5.62	98.04	107.99
1	B	239	GLU	N-CA-C	5.62	119.08	110.20
1	B	103	LEU	CD1-CG-CD2	-5.61	98.47	110.80
1	B	299	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	A	242	ASP	CA-C-O	5.59	128.50	120.51
1	B	290	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	4	GLU	CA-C-N	5.54	125.47	119.76
1	B	4	GLU	C-N-CA	5.54	125.47	119.76
1	B	69	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	B	180	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	B	235	ILE	N-CA-C	-5.51	107.91	113.20
1	B	12	THR	CA-CB-CG2	5.51	119.87	110.50
1	A	195	ASP	N-CA-C	5.50	117.35	111.36
1	B	313	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	274	TYR	CA-CB-CG	5.41	123.64	113.90
1	A	261	THR	CA-CB-OG1	-5.41	101.49	109.60
1	A	248	SER	N-CA-C	-5.37	101.91	109.96
1	B	182	VAL	N-CA-C	-5.36	101.23	107.61
1	B	103	LEU	N-CA-C	-5.36	99.79	108.52
1	B	32	ASP	N-CA-C	5.32	117.40	108.73
1	B	206	CYS	N-CA-CB	-5.31	103.93	111.84
1	A	55	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	B	240	ASN	O-C-N	-5.29	115.56	122.59
1	A	302	GLY	CA-C-N	5.27	127.60	120.38
1	A	302	GLY	C-N-CA	5.27	127.60	120.38
1	A	98	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	B	293	THR	CA-CB-CG2	5.24	119.41	110.50
1	B	67	THR	N-CA-C	-5.23	101.35	109.14
1	A	53	HIS	CB-CG-ND1	5.19	130.48	122.70
1	A	318	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	B	234	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	221	LEU	N-CA-C	-5.18	100.72	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	B	317	ASN	CB-CG-ND2	5.16	124.14	116.40
1	A	293	THR	O-C-N	-5.15	116.47	122.96
1	A	151	PHE	CA-CB-CG	5.14	118.94	113.80
1	A	279	ASP	N-CA-CB	-5.14	101.80	110.49
1	B	299	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	A	32	ASP	N-CA-C	5.13	116.98	108.20
1	B	148	GLN	CA-CB-CG	-5.13	103.84	114.10
1	A	189	TYR	N-CA-C	-5.13	102.41	110.36
1	B	276	LEU	N-CA-C	-5.10	101.40	109.76
1	A	134	THR	CA-CB-OG1	-5.08	101.97	109.60
1	B	3	ASP	N-CA-C	-5.07	100.15	108.41
1	B	90	GLN	N-CA-C	-5.06	100.91	108.96
1	B	166	LEU	CB-CG-CD1	-5.05	95.55	110.70
1	A	182	VAL	O-C-N	-5.02	115.38	121.10
1	A	223	GLY	CA-C-N	5.01	125.25	119.83
1	A	223	GLY	C-N-CA	5.01	125.25	119.83

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	2429	0	2255	42	0
1	B	2429	0	2255	36	0
2	A	38	0	55	22	0
2	B	38	0	55	20	0
3	A	54	0	0	0	0
3	B	56	0	0	0	0
All	All	5044	0	4620	113	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 12.

All (113) 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)
2:B:327:OZL:HD16	2:B:327:OZL:CD11	0.97	1.16
2:A:327:OZL:HD16	2:A:327:OZL:CD11	0.97	1.14
2:A:327:OZL:CD21	2:A:327:OZL:HD25	0.97	1.13
2:B:327:OZL:HD26	2:B:327:OZL:CD21	0.97	1.10
2:B:327:OZL:CD11	2:B:327:OZL:HD14	0.97	1.09
2:B:327:OZL:CD11	2:B:327:OZL:HD15	0.97	1.09
2:B:327:OZL:CD21	2:B:327:OZL:HD24	0.97	1.09
2:A:327:OZL:CD11	2:A:327:OZL:HD14	0.97	1.08
2:A:327:OZL:CD21	2:A:327:OZL:HD26	0.97	1.08
2:B:327:OZL:CD21	2:B:327:OZL:HD25	0.97	1.07
2:A:327:OZL:CD21	2:A:327:OZL:HD24	0.97	1.07
1:B:166:LEU:CB	1:B:166:LEU:CD1	2.34	1.06
2:A:327:OZL:CD11	2:A:327:OZL:HD15	0.97	1.04
1:B:166:LEU:CD1	1:B:166:LEU:HB2	1.96	0.95
2:A:327:OZL:HD25	2:A:327:OZL:CG1	2.04	0.87
2:A:327:OZL:HD16	2:A:327:OZL:CG1	2.05	0.86
2:A:327:OZL:HD26	2:A:327:OZL:CG1	2.04	0.86
2:B:327:OZL:HD24	2:B:327:OZL:CG1	2.06	0.86
2:A:327:OZL:HD14	2:A:327:OZL:CG1	2.05	0.86
2:A:327:OZL:HD24	2:A:327:OZL:CG1	2.04	0.86
2:A:327:OZL:HD25	2:A:327:OZL:HD24	1.58	0.86
2:A:327:OZL:HD16	2:A:327:OZL:HD14	1.58	0.85
2:A:327:OZL:HD15	2:A:327:OZL:CG1	2.05	0.85
2:B:327:OZL:HD16	2:B:327:OZL:HD15	1.58	0.85
2:B:327:OZL:HD25	2:B:327:OZL:CG1	2.06	0.85
2:A:327:OZL:HD16	2:A:327:OZL:HD15	1.58	0.85
2:B:327:OZL:HD14	2:B:327:OZL:HD15	1.58	0.85
2:B:327:OZL:HD26	2:B:327:OZL:HD25	1.58	0.85
2:B:327:OZL:HD15	2:B:327:OZL:CG1	2.07	0.85
2:A:327:OZL:HD26	2:A:327:OZL:HD24	1.58	0.85
2:B:327:OZL:HD16	2:B:327:OZL:HD14	1.58	0.85
2:A:327:OZL:HD25	2:A:327:OZL:HD26	1.58	0.85
2:B:327:OZL:HD26	2:B:327:OZL:HD24	1.58	0.85
2:B:327:OZL:HD14	2:B:327:OZL:CG1	2.07	0.85
2:B:327:OZL:HD26	2:B:327:OZL:CG1	2.06	0.84
2:B:327:OZL:HD16	2:B:327:OZL:CG1	2.06	0.84
2:B:327:OZL:HD24	2:B:327:OZL:HD25	1.58	0.84
2:A:327:OZL:HD14	2:A:327:OZL:HD15	1.58	0.83
1:A:69:GLN:HB3	1:A:84:LEU:HD13	1.76	0.66
1:B:172:SER:HA	1:B:175:TYR:CE1	2.30	0.66
1:A:41:PRO:HA	1:A:104:SER:OG	1.97	0.64
1:B:65:GLU:HB2	1:B:86:TYR:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HB2	1:B:163:SER:HB2	1.82	0.61
1:B:222:THR:HG23	1:B:289:MET:HB3	1.81	0.60
1:A:224:PRO:HB3	1:A:297:GLU:HG2	1.85	0.58
1:B:80:MET:HE2	1:B:104:SER:HB3	1.87	0.57
1:A:110:SER:O	1:A:113:TYR:HB3	2.05	0.57
1:A:194:LEU:O	1:A:209:GLY:HA2	2.07	0.55
1:B:30:ILE:HG13	2:B:327:OZL:H5'1	1.88	0.54
1:B:317:ASN:ND2	1:B:319:LYS:HB2	2.23	0.54
1:B:259:VAL:HG22	1:B:268:PRO:HB3	1.90	0.54
1:B:80:MET:C	1:B:80:MET:SD	2.91	0.53
1:A:183:PRO:HA	1:A:319:LYS:HG2	1.90	0.53
1:A:47:SER:OG	1:A:106:THR:HA	2.08	0.53
1:A:317:ASN:ND2	1:A:319:LYS:HB2	2.24	0.52
1:A:277:GLN:HA	1:A:281:SER:O	2.10	0.52
1:A:220:LEU:HA	1:A:304:VAL:HG23	1.91	0.51
1:B:41:PRO:HA	1:B:104:SER:OG	2.09	0.51
1:B:239:GLU:HG3	1:B:245:MET:HE2	1.91	0.51
1:B:181:TRP:HB3	1:B:319:LYS:HD3	1.92	0.51
1:A:276:LEU:O	1:A:282:CYS:HA	2.10	0.51
1:B:275:ILE:HG23	1:B:283:THR:O	2.11	0.50
1:B:1:ILE:HA	1:B:167:LEU:O	2.12	0.50
1:A:22:THR:O	1:A:61:SER:HA	2.12	0.50
1:A:48:LEU:HG	1:A:113:TYR:CD1	2.48	0.49
1:A:239:GLU:HG3	1:A:240:ASN:N	2.28	0.49
1:B:212:ALA:HA	1:B:299:TRP:O	2.12	0.48
1:A:219:SER:O	1:A:303:ASP:HB2	2.13	0.48
1:A:48:LEU:HG	1:A:113:TYR:CE1	2.48	0.48
1:A:289:MET:HG2	2:A:327:OZL:HD24	1.95	0.48
1:A:172:SER:HA	1:A:175:TYR:CE1	2.49	0.48
2:A:327:OZL:HD12	2:A:327:OZL:H5'2	1.95	0.48
1:A:14:TYR:OH	1:A:307:ARG:HD3	2.14	0.48
1:A:239:GLU:N	1:A:245:MET:HE2	2.29	0.48
1:A:161:SER:OG	1:B:26:ASP:HB3	2.14	0.47
1:A:1:ILE:HA	1:A:167:LEU:O	2.15	0.47
1:B:36:SER:OG	1:B:128:ILE:HG13	2.15	0.47
1:B:293:THR:HB	1:B:296:GLY:O	2.14	0.47
1:B:4:GLU:HG2	1:B:31:PHE:CZ	2.49	0.47
1:B:195:ASP:HB2	1:B:261:THR:O	2.15	0.46
1:B:220:LEU:HD12	1:B:287:GLU:HB2	1.97	0.46
1:B:7:GLU:O	1:B:14:TYR:HA	2.16	0.46
1:A:240:ASN:HB3	1:A:244:GLU:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HD12	1:A:286:PHE:HB3	1.98	0.45
1:A:239:GLU:H	1:A:245:MET:HE2	1.82	0.45
1:B:166:LEU:HB2	1:B:166:LEU:HD13	1.92	0.45
1:A:80:MET:HE2	1:A:104:SER:HB3	1.98	0.45
1:A:261:THR:HA	1:A:265:VAL:O	2.16	0.45
1:A:240:ASN:HB3	1:A:244:GLU:O	2.17	0.44
1:B:194:LEU:HD21	1:B:260:PHE:HD2	1.83	0.44
1:A:255:LEU:HA	1:A:256:PRO:HD3	1.67	0.44
1:B:191:GLN:HG3	1:B:213:ILE:HG22	1.99	0.43
1:B:224:PRO:HD2	1:B:299:TRP:CE2	2.53	0.43
1:A:204:ILE:HD12	1:A:231:ILE:HG12	2.01	0.43
1:B:240:ASN:HB3	1:B:244:GLU:HB2	2.01	0.43
1:B:77:THR:O	2:B:327:OZL:H3'2	2.19	0.42
1:B:43:VAL:HA	1:B:55:GLN:NE2	2.34	0.42
1:A:90:GLN:HA	1:A:94:ILE:O	2.19	0.42
1:B:134:THR:HG22	1:B:135:PRO:O	2.18	0.42
1:A:25:GLN:HA	1:B:160:ASP:HA	2.02	0.42
1:A:120:ILE:HD11	2:A:327:OZL:H4'2	2.02	0.42
1:A:4:GLU:HA	1:A:5:PRO:HD3	1.85	0.42
1:B:88:THR:HA	1:B:96:ASP:O	2.19	0.42
1:A:77:THR:O	2:A:327:OZL:H3'2	2.19	0.42
1:B:57:ASN:HA	1:B:58:PRO:HD2	1.85	0.42
1:A:303:ASP:O	1:A:307:ARG:HG3	2.20	0.41
1:B:293:THR:HG22	1:B:295:SER:H	1.84	0.41
1:A:220:LEU:HA	1:A:304:VAL:CG2	2.50	0.41
1:A:212:ALA:HA	1:A:299:TRP:O	2.21	0.41
1:A:275:ILE:CG2	1:A:282:CYS:HB3	2.51	0.41
1:A:197:ILE:HA	1:A:259:VAL:O	2.22	0.41
1:A:220:LEU:HB3	1:A:285:GLY:O	2.21	0.40
1:A:277:GLN:HG3	1:A:282:CYS:SG	2.62	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	324/326 (99%)	302 (93%)	21 (6%)	1 (0%)	36	65
1	B	324/326 (99%)	305 (94%)	14 (4%)	5 (2%)	8	28
All	All	648/652 (99%)	607 (94%)	35 (5%)	6 (1%)	14	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	ASP
1	A	188	GLY
1	B	188	GLY
1	B	225	THR
1	B	111	PHE
1	B	243	GLY

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	275/275 (100%)	246 (90%)	29 (10%)	6	22
1	B	275/275 (100%)	249 (90%)	26 (10%)	8	26
All	All	550/550 (100%)	495 (90%)	55 (10%)	7	24

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	74	THR
1	A	81	THR
1	A	83	ILE
1	A	95	SER
1	A	106	THR
1	A	127	SER

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Mol	Chain	Res	Type
1	A	147	SER
1	A	157	SER
1	A	163	SER
1	A	166	LEU
1	A	172	SER
1	A	176	THR
1	A	194	LEU
1	A	202	GLU
1	A	206	CYS
1	A	207	SER
1	A	222	THR
1	A	238	SER
1	A	240	ASN
1	A	245	MET
1	A	251	SER
1	A	272	SER
1	A	276	LEU
1	A	294	SER
1	A	295	SER
1	A	297	GLU
1	A	298	LEU
1	A	317	ASN
1	B	1	ILE
1	B	13	GLU
1	B	71	LEU
1	B	83	ILE
1	B	147	SER
1	B	166	LEU
1	B	167	LEU
1	B	170	ILE
1	B	176	THR
1	B	192	ILE
1	B	194	LEU
1	B	202	GLU
1	B	222	THR
1	B	226	SER
1	B	238	SER
1	B	239	GLU
1	B	250	SER
1	B	276	LEU
1	B	279	ASP
1	B	281	SER

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Mol	Chain	Res	Type
1	B	283	THR
1	B	293	THR
1	B	294	SER
1	B	295	SER
1	B	298	LEU
1	B	317	ASN

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	55	GLN
1	B	55	GLN
1	B	90	GLN
1	B	99	GLN
1	B	180	ASN
1	B	191	GLN
1	B	211	GLN
1	B	308	GLN
1	B	317	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0ZL	A	327	-	38,38,38	1.09	3 (7%)	46,50,50	1.60	6 (13%)
2	0ZL	B	327	-	38,38,38	1.09	2 (5%)	46,50,50	1.69	11 (23%)

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	0ZL	A	327	-	-	3/47/55/55	0/1/1/1
2	0ZL	B	327	-	-	6/47/55/55	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	327	0ZL	O2-C1	4.54	1.44	1.35
2	A	327	0ZL	O2-C1	3.90	1.43	1.35
2	A	327	0ZL	O2-C4	-3.23	1.36	1.46
2	B	327	0ZL	O2-C4	-2.69	1.38	1.46
2	A	327	0ZL	C7'-C1'	-2.20	1.49	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	327	0ZL	C4-O2-C1	5.86	127.02	116.06
2	B	327	0ZL	C4-O2-C1	4.10	123.73	116.06
2	B	327	0ZL	O2-C1-N	3.93	118.86	110.45
2	B	327	0ZL	C5-C41-C31	3.56	119.77	114.82
2	A	327	0ZL	O2-C1-N	3.01	116.90	110.45
2	B	327	0ZL	C2-CA1-N1	-2.92	103.22	111.11
2	B	327	0ZL	CG-CB-CA	2.75	122.77	115.40
2	A	327	0ZL	CG1-CB1-CA1	2.66	122.54	115.40
2	B	327	0ZL	C3'-C2'-C1'	-2.59	106.62	112.08
2	A	327	0ZL	C2-CA1-N1	-2.58	104.14	111.11
2	B	327	0ZL	O2-C1-O1	-2.56	119.35	124.26
2	B	327	0ZL	C-CA-N	-2.43	104.54	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	327	0ZL	C7'-C11-N2	-2.26	107.29	110.20
2	B	327	0ZL	C4'-C3'-C2'	-2.17	106.96	111.42
2	B	327	0ZL	C7'-C11-N2	-2.14	107.45	110.20
2	B	327	0ZL	O31-C31-C41	2.13	113.42	109.15
2	A	327	0ZL	CA-C-N1	-2.10	112.16	116.63

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	327	0ZL	C2-CA1-CB1-CG1
2	B	327	0ZL	CA1-CB1-CG1-CD11
2	B	327	0ZL	CA1-CB1-CG1-CD21
2	B	327	0ZL	N1-CA1-CB1-CG1
2	A	327	0ZL	N2-C2-CA1-N1
2	A	327	0ZL	O3-C2-CA1-N1
2	B	327	0ZL	N2-C2-CA1-N1
2	A	327	0ZL	C2-CA1-CB1-CG1
2	B	327	0ZL	O3-C2-CA1-N1

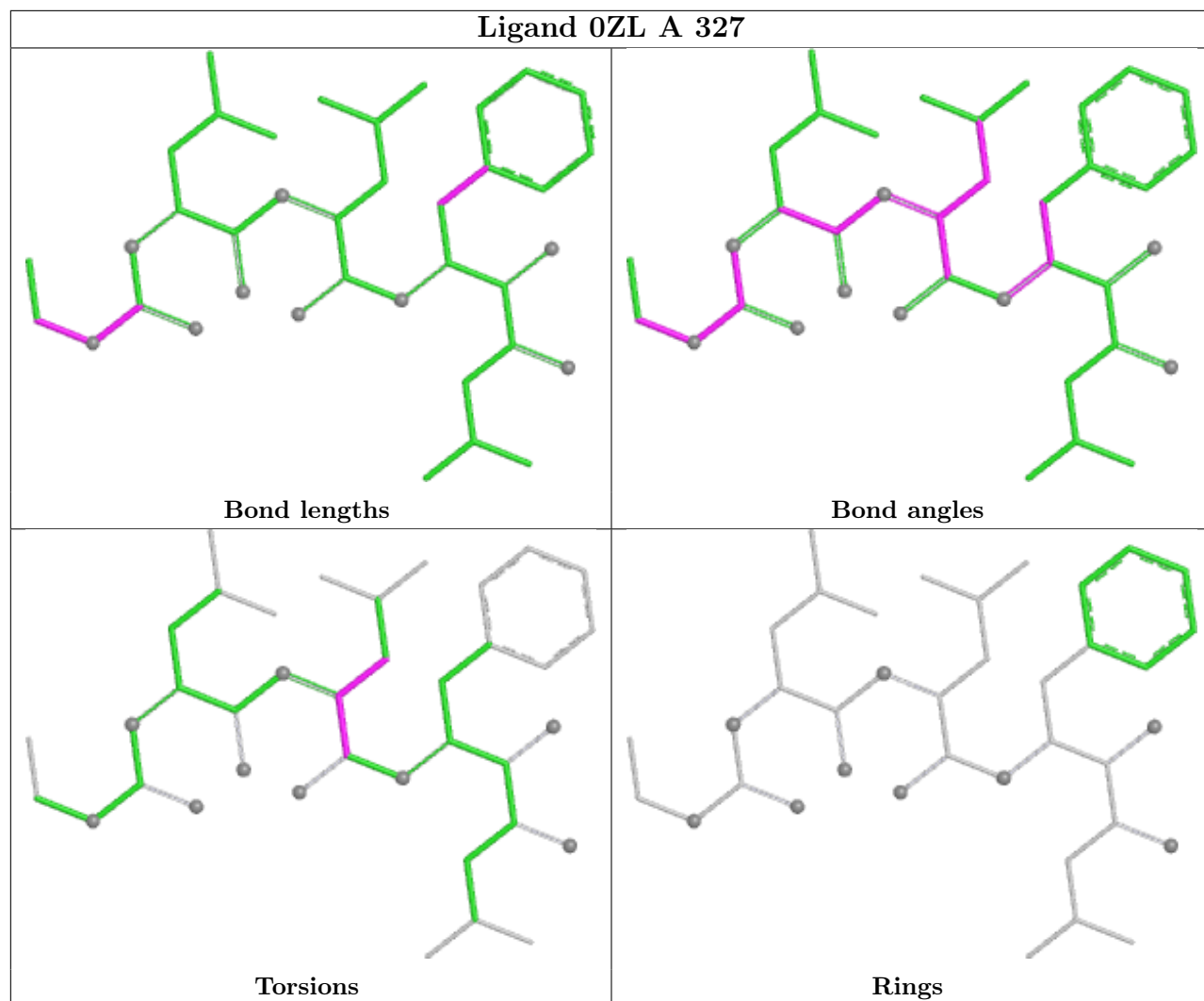
There are no ring outliers.

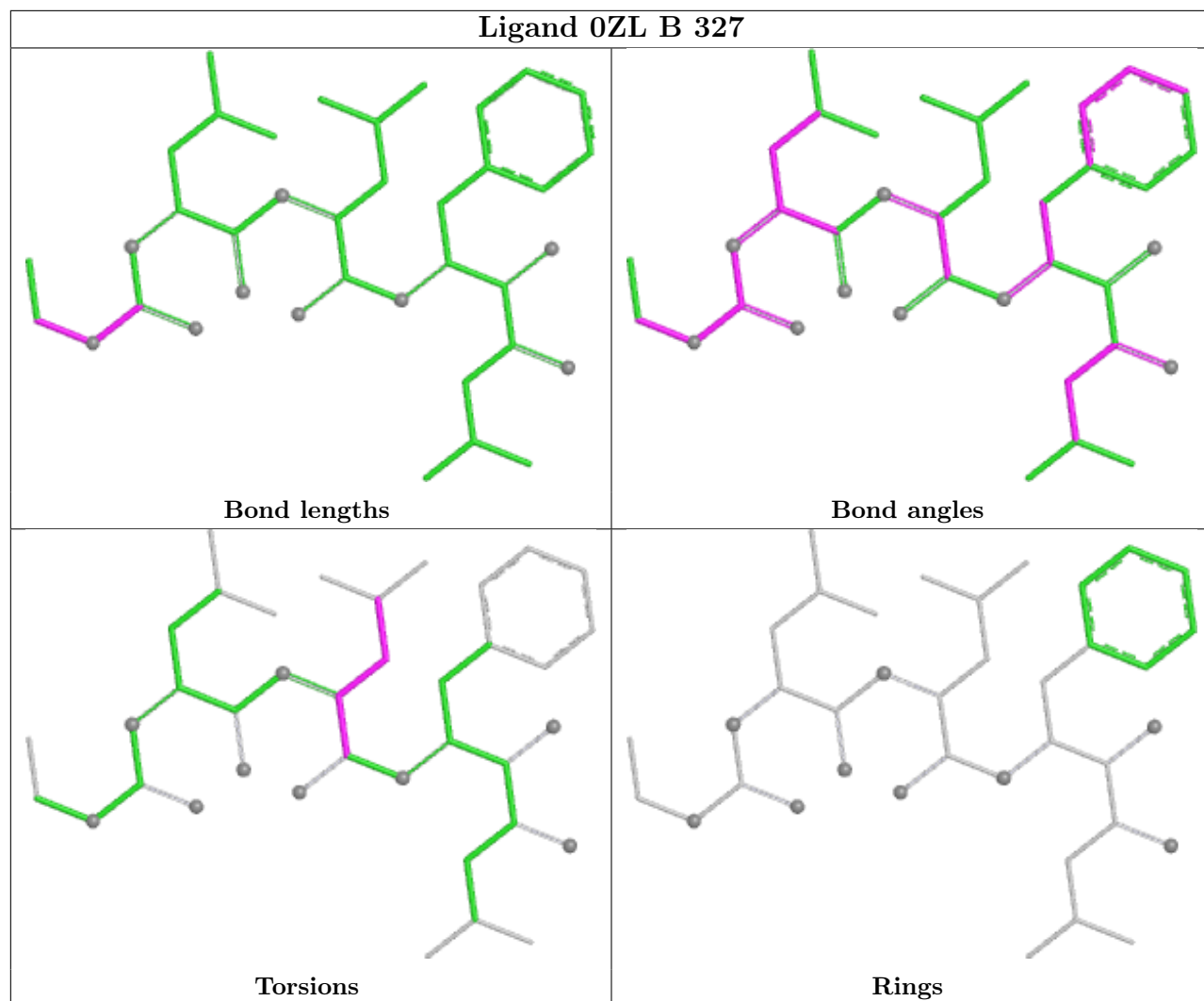
2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	327	0ZL	22	0
2	B	327	0ZL	20	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.

Ligand 0ZL A 327





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	326/326 (100%)	-1.07	1 (0%) 90 87	2, 8, 38, 71	2 (0%)
1	B	326/326 (100%)	-1.07	1 (0%) 90 87	2, 6, 39, 81	2 (0%)
All	All	652/652 (100%)	-1.07	2 (0%) 90 87	2, 7, 39, 81	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	2.6
1	A	243	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

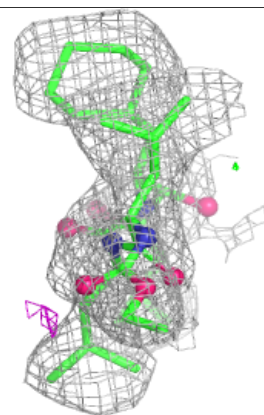
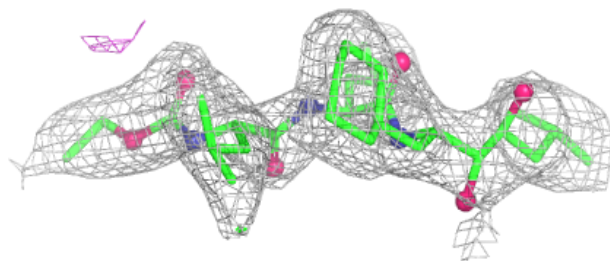
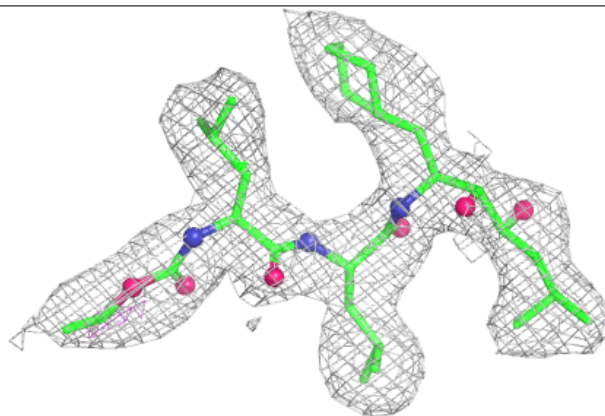
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0ZL	A	327	38/38	0.97	0.05	2,8,13,14	0
2	0ZL	B	327	38/38	0.97	0.05	2,3,11,16	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.

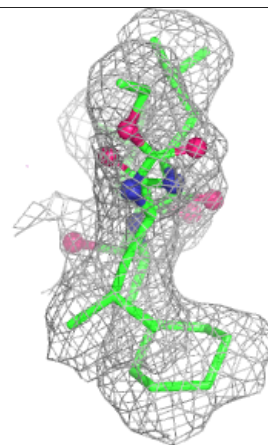
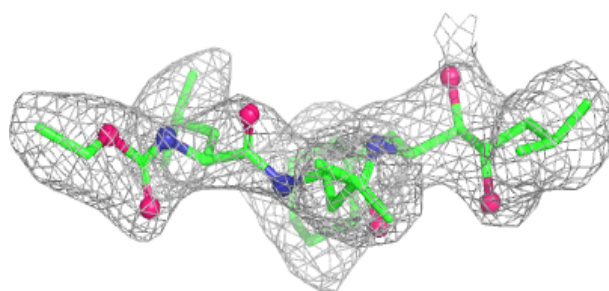
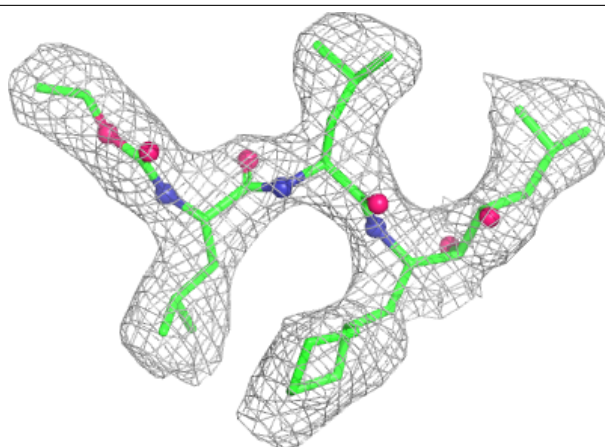
Electron density around 0ZL A 327:

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



Electron density around 0ZL B 327:

$2mF_o-DF_c$ (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.