



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:51 AM UTC

PDB ID : 9LPL / pdb_00009lpl
Title : E. coli FabF mutant -C163Q
Authors : Chen, L.; Huang, Y.
Deposited on : 2025-01-25
Resolution : 2.70 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

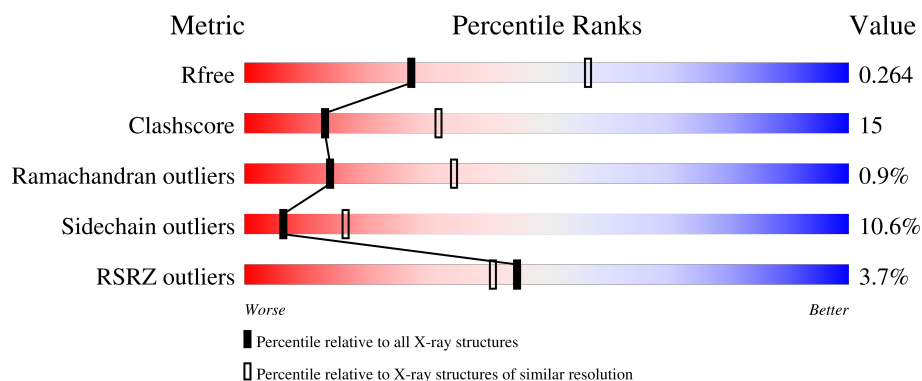
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

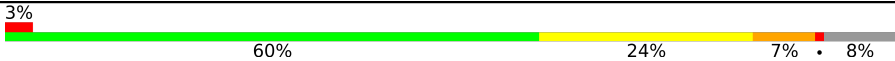
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	443	
1	B	443	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6120 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 3-oxoacyl-[acyl-carrier-protein] synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			2990	1865	525	584	16			
1	B	410	Total	C	N	O	S	0	0	0
			2999	1871	527	585	16			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	HIS	-	expression tag	UNP P0AAI5
A	-16	HIS	-	expression tag	UNP P0AAI5
A	-15	HIS	-	expression tag	UNP P0AAI5
A	-14	HIS	-	expression tag	UNP P0AAI5
A	-13	HIS	-	expression tag	UNP P0AAI5
A	-12	HIS	-	expression tag	UNP P0AAI5
A	-11	SER	-	expression tag	UNP P0AAI5
A	-10	SER	-	expression tag	UNP P0AAI5
A	-9	GLY	-	expression tag	UNP P0AAI5
A	-8	LEU	-	expression tag	UNP P0AAI5
A	-7	VAL	-	expression tag	UNP P0AAI5
A	-6	PRO	-	expression tag	UNP P0AAI5
A	-5	ARG	-	expression tag	UNP P0AAI5
A	-4	GLY	-	expression tag	UNP P0AAI5
A	-3	SER	-	expression tag	UNP P0AAI5
A	-2	HIS	-	expression tag	UNP P0AAI5
A	-1	MET	-	expression tag	UNP P0AAI5
A	0	VAL	-	expression tag	UNP P0AAI5
A	163	GLN	CYS	engineered mutation	UNP P0AAI5
A	413	LYS	-	expression tag	UNP P0AAI5
A	414	LEU	-	expression tag	UNP P0AAI5
A	415	ALA	-	expression tag	UNP P0AAI5
A	416	ALA	-	expression tag	UNP P0AAI5
A	417	ALA	-	expression tag	UNP P0AAI5
A	418	LEU	-	expression tag	UNP P0AAI5

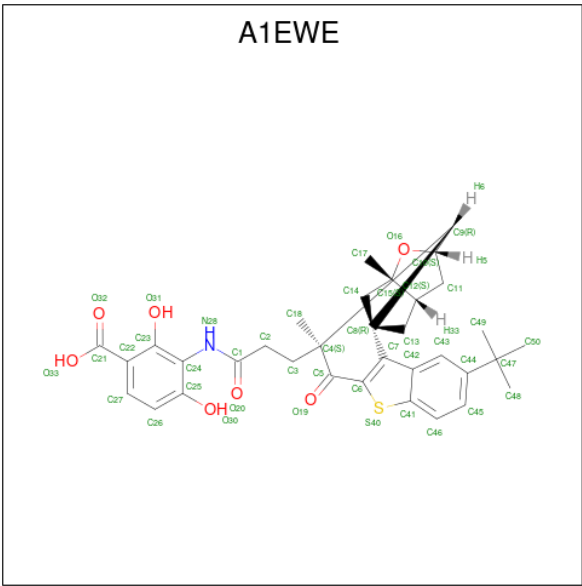
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Chain	Residue	Modelled	Actual	Comment	Reference
A	419	GLU	-	expression tag	UNP P0AAI5
A	420	HIS	-	expression tag	UNP P0AAI5
A	421	HIS	-	expression tag	UNP P0AAI5
A	422	HIS	-	expression tag	UNP P0AAI5
A	423	HIS	-	expression tag	UNP P0AAI5
A	424	HIS	-	expression tag	UNP P0AAI5
A	425	HIS	-	expression tag	UNP P0AAI5
B	-17	HIS	-	expression tag	UNP P0AAI5
B	-16	HIS	-	expression tag	UNP P0AAI5
B	-15	HIS	-	expression tag	UNP P0AAI5
B	-14	HIS	-	expression tag	UNP P0AAI5
B	-13	HIS	-	expression tag	UNP P0AAI5
B	-12	HIS	-	expression tag	UNP P0AAI5
B	-11	SER	-	expression tag	UNP P0AAI5
B	-10	SER	-	expression tag	UNP P0AAI5
B	-9	GLY	-	expression tag	UNP P0AAI5
B	-8	LEU	-	expression tag	UNP P0AAI5
B	-7	VAL	-	expression tag	UNP P0AAI5
B	-6	PRO	-	expression tag	UNP P0AAI5
B	-5	ARG	-	expression tag	UNP P0AAI5
B	-4	GLY	-	expression tag	UNP P0AAI5
B	-3	SER	-	expression tag	UNP P0AAI5
B	-2	HIS	-	expression tag	UNP P0AAI5
B	-1	MET	-	expression tag	UNP P0AAI5
B	0	VAL	-	expression tag	UNP P0AAI5
B	163	GLN	CYS	engineered mutation	UNP P0AAI5
B	413	LYS	-	expression tag	UNP P0AAI5
B	414	LEU	-	expression tag	UNP P0AAI5
B	415	ALA	-	expression tag	UNP P0AAI5
B	416	ALA	-	expression tag	UNP P0AAI5
B	417	ALA	-	expression tag	UNP P0AAI5
B	418	LEU	-	expression tag	UNP P0AAI5
B	419	GLU	-	expression tag	UNP P0AAI5
B	420	HIS	-	expression tag	UNP P0AAI5
B	421	HIS	-	expression tag	UNP P0AAI5
B	422	HIS	-	expression tag	UNP P0AAI5
B	423	HIS	-	expression tag	UNP P0AAI5
B	424	HIS	-	expression tag	UNP P0AAI5
B	425	HIS	-	expression tag	UNP P0AAI5

- Molecule 2 is 3-(3-((2S,3S,5S,5aR,6S,12cR)-11-(tert-butyl)-2,6-dimethyl-7-oxo-1,2,3,4,5,5a,6,7-octahydro-2,5-epoxy-3,12c-methanobenzo[b]cyclohepta[5,6]benzo[1,2-d]thiophen-6-yl)propanamido)-2,4-dihydroxybenzoic acid (CCD ID: A1EWE) (formula: C₃₄H₃₇NO₇S) (labeled

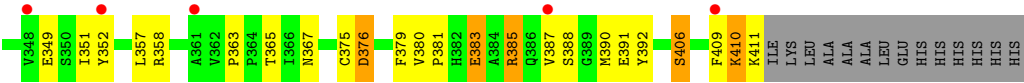
as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			43	34	1	7	1		
2	B	1	Total	C	N	O	S	0	0
			43	34	1	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	21	Total	O	0	0
			21	21		



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.76Å 79.76Å 299.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.27 – 2.70 33.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.9 (33.27-2.70) 98.9 (33.27-2.70)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.204 , 0.263 0.209 , 0.264	Depositor DCC
R_{free} test set	1503 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6120	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.2306e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1EWE

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	1.01	0/3042	1.79	55/4115 (1.3%)
1	B	1.03	1/3051 (0.0%)	1.85	69/4126 (1.7%)
All	All	1.02	1/6093 (0.0%)	1.82	124/8241 (1.5%)

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	5
1	B	0	5
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	HIS	CG-CD2	-5.16	1.30	1.35

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	CA-CB-OG1	-15.52	86.33	109.60
1	B	19	THR	CA-CB-OG1	-12.95	90.17	109.60
1	B	226	ARG	CB-CA-C	-12.35	85.84	110.42
1	A	226	ARG	CB-CA-C	-12.25	86.05	110.42
1	B	376	ASP	CA-CB-CG	11.30	123.90	112.60
1	B	305	THR	CA-CB-OG1	-11.10	92.95	109.60
1	B	122	MET	CG-SD-CE	10.93	124.96	100.90
1	A	31	GLN	N-CA-CB	10.17	125.41	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CA-CB-CG	9.71	122.31	112.60
1	B	338	THR	CA-CB-OG1	-9.38	95.54	109.60
1	A	305	THR	CA-CB-OG1	-8.85	96.32	109.60
1	A	118	HIS	CA-CB-CG	-8.81	104.98	113.80
1	A	122	MET	CG-SD-CE	8.69	120.01	100.90
1	B	67	GLN	CB-CA-C	-8.67	96.40	110.79
1	B	324	GLU	CB-CA-C	8.62	126.48	110.70
1	A	181	ASP	CA-CB-CG	8.07	120.67	112.60
1	B	265	ASP	CA-CB-CG	8.04	120.64	112.60
1	B	409	PHE	CA-CB-CG	-7.97	105.83	113.80
1	A	25	LYS	CB-CA-C	7.62	124.65	110.70
1	A	320	THR	CA-CB-OG1	-7.62	98.17	109.60
1	A	172	HIS	CA-CB-CG	-7.47	106.33	113.80
1	B	231	LEU	N-CA-CB	-7.34	98.91	109.85
1	B	363	PRO	CB-CA-C	7.31	119.84	110.92
1	A	231	LEU	N-CA-CB	-7.17	99.43	109.97
1	B	31	GLN	N-CA-CB	6.99	121.55	110.23
1	B	69	LYS	CB-CA-C	-6.88	98.93	110.56
1	A	25	LYS	CA-CB-CG	6.87	127.83	114.10
1	B	38	ASP	CA-CB-CG	6.73	119.33	112.60
1	B	141	MET	CG-SD-CE	-6.67	86.22	100.90
1	B	47	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	141	MET	CG-SD-CE	-6.50	86.60	100.90
1	A	328	ARG	CB-CA-C	6.49	123.61	110.38
1	B	20	VAL	N-CA-CB	6.46	117.66	110.62
1	A	151	GLY	O-C-N	-6.43	117.30	122.51
1	A	186	VAL	N-CA-CB	6.43	118.22	110.31
1	B	320	THR	CA-CB-OG1	-6.41	99.98	109.60
1	B	328	ARG	CB-CA-C	6.41	122.71	109.95
1	B	19	THR	CA-C-O	-6.39	114.61	121.45
1	A	225	GLU	CB-CA-C	-6.37	99.95	110.72
1	A	119	THR	CA-CB-OG1	6.37	119.15	109.60
1	B	96	ASN	CB-CA-C	6.31	123.18	109.99
1	B	186	VAL	N-CA-CB	6.30	118.06	110.31
1	B	99	ARG	CG-CD-NE	6.28	125.81	112.00
1	B	41	ASP	CA-CB-CG	6.26	118.86	112.60
1	A	303	HIS	N-CA-C	-6.24	104.11	111.03
1	A	19	THR	CA-CB-OG1	-6.19	100.32	109.60
1	A	381	PRO	CA-C-O	-6.15	114.33	121.34
1	B	185	MET	CB-CA-C	-6.14	103.08	110.94
1	A	139	VAL	N-CA-CB	-6.10	99.72	110.77
1	B	303	HIS	N-CA-C	-6.03	104.34	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	GLU	CB-CG-CD	6.01	122.83	112.60
1	B	172	HIS	CA-CB-CG	-5.98	107.82	113.80
1	B	116	GLU	CB-CG-CD	-5.97	102.44	112.60
1	A	383	GLU	CB-CA-C	-5.96	97.98	109.37
1	A	54	LYS	N-CA-CB	5.96	119.89	110.23
1	B	202	PHE	CB-CA-C	5.88	120.20	110.90
1	B	376	ASP	CB-CA-C	5.87	123.07	110.21
1	A	409	PHE	CA-CB-CG	-5.79	108.01	113.80
1	A	40	PHE	CA-C-O	-5.78	115.26	121.45
1	A	158	SER	CA-C-N	-5.77	114.65	122.91
1	A	158	SER	C-N-CA	-5.77	114.65	122.91
1	A	272	PRO	CB-CA-C	-5.77	103.88	110.92
1	A	386	GLN	N-CA-CB	-5.72	101.76	110.45
1	B	68	ARG	CG-CD-NE	-5.62	99.63	112.00
1	A	355	LEU	CA-C-N	5.57	127.69	120.44
1	A	355	LEU	C-N-CA	5.57	127.69	120.44
1	B	97	ALA	N-CA-C	5.57	118.07	111.33
1	B	37	ILE	CA-C-N	5.53	132.20	122.42
1	B	37	ILE	C-N-CA	5.53	132.20	122.42
1	B	175	ARG	CA-C-N	5.51	127.50	120.56
1	B	175	ARG	C-N-CA	5.51	127.50	120.56
1	A	367	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	19	THR	CA-CB-CG2	5.43	119.73	110.50
1	B	319	LYS	CB-CG-CD	5.43	123.78	111.30
1	B	68	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	3	ARG	CB-CG-CD	5.42	123.76	111.30
1	B	98	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	134	VAL	N-CA-CB	5.42	118.79	111.21
1	B	249	ARG	CB-CG-CD	5.40	123.73	111.30
1	A	64	ARG	CA-CB-CG	5.40	124.90	114.10
1	B	358	ARG	CA-C-O	-5.40	114.82	120.55
1	B	216	GLN	N-CA-C	-5.37	106.72	113.28
1	B	161	THR	N-CA-C	-5.36	104.01	110.44
1	B	68	ARG	CB-CA-C	-5.35	99.78	110.42
1	B	383	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	48	LYS	N-CA-CB	-5.29	102.70	111.49
1	B	118	HIS	CA-CB-CG	-5.29	108.51	113.80
1	B	270	THR	OG1-CB-CG2	-5.28	98.75	109.30
1	A	243	TYR	CB-CA-C	5.25	119.12	110.88
1	B	142	VAL	N-CA-CB	5.25	117.29	110.57
1	A	289	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	82	VAL	CA-CB-CG1	5.24	119.31	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	365	THR	CA-CB-OG1	-5.23	101.75	109.60
1	B	94	GLU	CA-C-N	5.23	127.24	120.44
1	B	94	GLU	C-N-CA	5.23	127.24	120.44
1	A	358	ARG	CD-NE-CZ	5.22	131.71	124.40
1	A	104	ILE	O-C-N	5.21	129.03	123.03
1	A	376	ASP	CB-CA-C	5.21	120.79	110.42
1	B	134	VAL	N-CA-CB	5.21	118.50	111.21
1	B	213	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	383	GLU	N-CA-CB	5.21	119.89	110.83
1	A	139	VAL	N-CA-C	5.18	117.56	111.09
1	B	94	GLU	CB-CA-C	-5.17	102.77	110.88
1	B	249	ARG	N-CA-CB	5.16	118.39	110.70
1	A	191	GLU	CB-CA-C	-5.15	98.96	109.94
1	B	206	ARG	CB-CA-C	5.15	118.63	111.63
1	B	196	PRO	CB-CA-C	5.14	120.04	111.56
1	A	54	LYS	CB-CG-CD	5.13	123.10	111.30
1	A	264	SER	CA-C-N	5.12	127.57	120.29
1	A	264	SER	C-N-CA	5.12	127.57	120.29
1	A	331	VAL	N-CA-CB	-5.09	103.09	111.44
1	B	239	VAL	N-CA-CB	-5.08	105.06	111.41
1	A	175	ARG	CA-C-N	5.08	126.96	120.56
1	A	175	ARG	C-N-CA	5.08	126.96	120.56
1	A	3	ARG	N-CA-CB	5.07	119.12	110.50
1	A	224	LYS	CG-CD-CE	5.06	122.94	111.30
1	B	338	THR	OG1-CB-CG2	5.06	119.41	109.30
1	B	221	PRO	O-C-N	5.04	129.28	122.89
1	A	145	HIS	CA-CB-CG	-5.03	108.77	113.80
1	B	211	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	B	48	LYS	CG-CD-CE	5.02	122.85	111.30
1	B	303	HIS	CB-CA-C	5.02	118.73	110.95
1	A	338	THR	N-CA-CB	-5.01	102.81	110.33
1	B	37	ILE	O-C-N	5.01	128.37	122.81

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	ARG	Sidechain
1	A	220	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	288	ARG	Sidechain
1	A	4	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	206	ARG	Sidechain
1	B	220	ARG	Sidechain
1	B	226	ARG	Sidechain
1	B	376	ASP	Peptide
1	B	99	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	2990	0	2949	86	0
1	B	2999	0	2962	104	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
3	A	24	0	0	3	0
3	B	21	0	0	4	0
All	All	6120	0	5911	177	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 15.

All (177) 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:135:PRO:HA	1:B:141:MET:CE	1.99	0.93
1:A:135:PRO:HA	1:A:141:MET:CE	2.02	0.89
1:A:135:PRO:HA	1:A:141:MET:HE3	1.58	0.86
1:B:387:VAL:HG22	1:B:388:SER:H	1.40	0.84
1:B:349:GLU:OE1	3:B:601:HOH:O	1.95	0.84
1:A:338:THR:HG22	1:A:339:GLY:O	1.81	0.81
1:A:122:MET:CB	1:B:122:MET:HE1	2.11	0.80
1:A:122:MET:HB2	1:B:122:MET:HE1	1.64	0.77
1:B:135:PRO:HA	1:B:141:MET:HE3	1.64	0.77
1:B:385:ARG:HH11	1:B:385:ARG:HB2	1.49	0.76
1:A:111:LEU:O	1:A:115:GLU:HG3	1.86	0.75
1:A:226:ARG:HH11	1:A:226:ARG:HG3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HG3	1:B:226:ARG:HH11	1.50	0.74
1:B:135:PRO:HA	1:B:141:MET:HE2	1.69	0.74
1:B:335:LYS:HA	1:B:338:THR:HG22	1.71	0.73
1:A:135:PRO:CA	1:A:141:MET:HE3	2.18	0.72
1:A:122:MET:HG3	1:B:122:MET:CE	2.20	0.72
1:B:88:SER:O	1:B:249:ARG:NH2	2.22	0.71
1:B:108:ILE:HG21	1:B:111:LEU:HD11	1.74	0.69
1:A:31:GLN:O	1:A:337:MET:HB3	1.95	0.67
1:A:93:THR:HG23	3:A:605:HOH:O	1.95	0.66
1:A:241:GLU:OE1	1:A:249:ARG:HD3	1.96	0.65
1:B:241:GLU:OE2	1:B:249:ARG:NH1	2.30	0.64
1:B:2:LYS:N	3:B:604:HOH:O	2.31	0.64
1:A:122:MET:HG3	1:B:122:MET:HE1	1.79	0.63
1:B:135:PRO:CA	1:B:141:MET:HE3	2.27	0.63
1:B:60:ASP:OD1	1:B:61:ILE:HD12	1.99	0.62
1:B:99:ARG:NH1	1:B:180:GLY:O	2.32	0.62
1:A:175:ARG:NH2	1:B:181:ASP:OD2	2.32	0.61
1:A:71:ASP:HA	1:A:113:LEU:HD22	1.83	0.61
1:A:358:ARG:HH21	1:A:359:ASP:CG	2.07	0.61
1:A:122:MET:CG	1:B:122:MET:HE1	2.31	0.61
1:B:150:TYR:HB3	1:B:152:LEU:HD21	1.84	0.60
1:B:222:TRP:CE2	1:B:379:PHE:CE1	2.89	0.60
1:A:69:LYS:HG2	1:A:132:PHE:CD1	2.36	0.60
1:B:387:VAL:HG22	1:B:388:SER:N	2.14	0.60
1:B:268:HIS:CD2	1:B:270:THR:H	2.20	0.60
1:A:135:PRO:HA	1:A:141:MET:HE2	1.81	0.59
1:A:222:TRP:CE2	1:A:379:PHE:CE1	2.91	0.59
1:B:99:ARG:HH21	1:B:99:ARG:HG3	1.68	0.59
1:A:71:ASP:CA	1:A:113:LEU:HD22	2.33	0.59
1:A:100:ILE:CG2	1:A:152:LEU:HD22	2.33	0.58
1:A:248:LYS:HG3	1:A:248:LYS:O	2.02	0.58
1:B:84:ALA:HB1	1:B:239:VAL:HG23	1.87	0.57
1:B:103:ALA:HB3	1:B:173:ALA:HB2	1.86	0.57
1:A:268:HIS:CD2	1:A:270:THR:H	2.23	0.57
1:B:238:LEU:HD12	1:B:240:LEU:HD21	1.87	0.56
1:A:151:GLY:HA2	1:B:266:ALA:HB1	1.87	0.56
1:B:380:VAL:N	1:B:381:PRO:HD3	2.21	0.56
1:B:223:ASP:O	1:B:226:ARG:HG3	2.06	0.56
1:B:104:ILE:HG21	1:B:142:VAL:CG1	2.36	0.55
1:B:238:LEU:N	1:B:238:LEU:HD23	2.21	0.55
1:A:6:VAL:HG11	1:A:243:TYR:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HG22	1:A:108:ILE:O	2.07	0.55
1:B:135:PRO:CB	1:B:141:MET:HE3	2.37	0.54
1:A:135:PRO:CB	1:A:141:MET:HE3	2.37	0.54
1:B:208:LEU:O	1:B:209:SER:C	2.50	0.54
1:B:104:ILE:HG21	1:B:142:VAL:HG12	1.90	0.54
1:A:133:PHE:O	1:A:137:THR:HB	2.07	0.54
1:B:241:GLU:OE1	1:B:249:ARG:HD3	2.08	0.54
1:A:299:TYR:CD1	1:A:362:VAL:HG11	2.43	0.54
1:A:392:TYR:CE1	1:A:410:LYS:HG3	2.43	0.53
1:B:206:ARG:HA	1:B:206:ARG:NH1	2.24	0.53
1:A:305:THR:O	1:A:306:SER:CB	2.55	0.53
1:B:241:GLU:CD	1:B:249:ARG:HH11	2.16	0.53
1:B:211:ARG:HG2	1:B:211:ARG:O	2.09	0.52
1:A:133:PHE:HD2	1:B:201:GLY:HA3	1.74	0.52
1:B:285:ASN:OD1	1:B:288:ARG:NH1	2.43	0.52
1:B:305:THR:O	1:B:306:SER:CB	2.54	0.52
1:A:275:ASN:HD22	1:A:277:ALA:H	1.57	0.52
1:B:99:ARG:HD3	3:B:615:HOH:O	2.09	0.52
1:A:237:MET:C	1:A:238:LEU:HD23	2.35	0.51
1:B:8:THR:O	1:B:88:SER:HA	2.11	0.51
1:A:118:HIS:CD2	1:B:118:HIS:HD2	2.29	0.51
1:A:223:ASP:O	1:A:226:ARG:HG3	2.10	0.51
1:B:147:THR:O	1:B:151:GLY:N	2.44	0.51
1:B:99:ARG:HH22	1:B:183:ASP:CG	2.20	0.50
1:B:357:LEU:O	1:B:411:LYS:NZ	2.44	0.50
1:A:164:THR:HG22	1:A:164:THR:O	2.11	0.50
1:B:132:PHE:O	1:B:136:SER:HB3	2.11	0.50
1:B:164:THR:HG22	1:B:164:THR:O	2.10	0.50
1:A:268:HIS:HD2	1:A:270:THR:H	1.59	0.50
1:A:12:MET:HE2	1:A:351:ILE:HG21	1.94	0.50
1:A:135:PRO:O	1:A:141:MET:HG3	2.12	0.50
1:B:60:ASP:OD1	1:B:61:ILE:CD1	2.59	0.50
1:B:7:VAL:HG11	1:B:10:LEU:HD21	1.94	0.49
1:B:298:GLY:HA3	1:B:390:MET:HG3	1.92	0.49
1:A:6:VAL:HG11	1:A:243:TYR:CD1	2.47	0.49
1:A:269:MET:C	3:A:603:HOH:O	2.54	0.49
1:A:6:VAL:HG22	1:A:241:GLU:O	2.12	0.49
1:B:392:TYR:CE1	1:B:410:LYS:HG3	2.47	0.49
1:B:281:LEU:HD22	1:B:285:ASN:ND2	2.27	0.49
1:B:48:LYS:N	1:B:212:ASN:OD1	2.43	0.49
1:A:132:PHE:O	1:A:133:PHE:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:MET:CE	1:B:145:HIS:CE1	2.95	0.48
1:A:147:THR:O	1:A:151:GLY:N	2.47	0.48
1:A:6:VAL:O	1:A:6:VAL:HG23	2.12	0.48
1:A:75:GLN:O	1:A:79:VAL:HG13	2.14	0.48
1:A:299:TYR:CE1	1:A:362:VAL:CG1	2.96	0.48
1:B:150:TYR:CB	1:B:152:LEU:HD21	2.43	0.48
1:A:110:GLY:O	1:A:114:ILE:HD12	2.14	0.48
1:B:15:PRO:HA	1:B:52:LEU:O	2.14	0.47
1:B:69:LYS:HG2	1:B:132:PHE:CD1	2.48	0.47
1:A:118:HIS:CE1	1:A:121:LEU:HD23	2.48	0.47
1:B:6:VAL:HG11	1:B:243:TYR:CD1	2.50	0.47
1:B:99:ARG:NH2	1:B:183:ASP:CG	2.73	0.47
1:B:380:VAL:N	1:B:381:PRO:CD	2.78	0.47
1:B:385:ARG:HB2	1:B:385:ARG:NH1	2.24	0.47
1:A:52:LEU:O	1:A:54:LYS:NZ	2.48	0.47
1:A:145:HIS:O	1:A:149:MET:HG3	2.15	0.47
1:A:301:ASN:ND2	1:A:301:ASN:C	2.73	0.47
1:B:99:ARG:HH21	1:B:99:ARG:CG	2.28	0.47
1:B:214:ASN:C	1:B:214:ASN:HD22	2.24	0.46
1:B:73:PHE:CE2	1:B:109:GLY:HA2	2.51	0.46
1:B:12:MET:CE	1:B:351:ILE:HG21	2.45	0.46
1:B:99:ARG:HD2	1:B:99:ARG:HA	1.70	0.46
1:A:93:THR:CG2	3:A:605:HOH:O	2.57	0.46
1:A:12:MET:CE	1:A:351:ILE:HG21	2.46	0.45
1:B:220:ARG:N	1:B:221:PRO:HD3	2.30	0.45
1:B:217:ALA:HA	1:B:367:ASN:ND2	2.31	0.45
1:B:4:ARG:O	1:B:242:GLU:HA	2.16	0.45
1:B:99:ARG:NH2	1:B:183:ASP:OD2	2.50	0.44
1:A:336:SER:HB2	1:A:366:ILE:HG13	1.99	0.44
1:A:409:PHE:CD2	1:A:409:PHE:N	2.85	0.44
1:A:15:PRO:HA	1:A:52:LEU:O	2.17	0.44
1:A:61:ILE:HD13	1:A:82:VAL:HG11	2.00	0.44
1:B:244:GLU:HB3	1:B:248:LYS:NZ	2.32	0.44
1:A:301:ASN:C	1:A:301:ASN:HD22	2.25	0.44
1:A:299:TYR:CD1	1:A:362:VAL:CG1	3.01	0.44
1:A:45:TYR:OH	1:A:196:PRO:HB3	2.18	0.44
1:B:145:HIS:O	1:B:149:MET:HG3	2.17	0.44
1:A:118:HIS:HD2	1:B:118:HIS:HD2	1.65	0.43
1:B:103:ALA:O	1:B:187:ALA:HA	2.17	0.43
1:B:105:GLY:HA3	1:B:169:ASN:HD21	1.82	0.43
1:A:220:ARG:HH11	1:A:223:ASP:CG	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:O	1:A:88:SER:HA	2.17	0.43
1:B:226:ARG:HE	1:B:308:PRO:HA	1.84	0.43
1:B:31:GLN:O	1:B:337:MET:HB3	2.18	0.43
1:B:301:ASN:HD22	1:B:301:ASN:C	2.26	0.43
1:A:100:ILE:HG22	1:A:152:LEU:HD22	1.97	0.43
1:A:197:LEU:HD13	1:A:197:LEU:HA	1.87	0.43
1:A:260:PHE:HA	1:A:406:SER:O	2.18	0.43
1:B:70:MET:HE1	1:B:145:HIS:CE1	2.54	0.43
1:B:281:LEU:HD22	1:B:285:ASN:HD21	1.84	0.43
1:A:161:THR:HG21	1:B:157:ILE:HA	2.01	0.43
1:B:140:ASN:HA	1:B:158:SER:OG	2.18	0.43
1:B:260:PHE:HA	1:B:406:SER:O	2.19	0.43
1:A:201:GLY:HA3	1:B:133:PHE:HD2	1.84	0.42
1:A:238:LEU:HD23	1:A:238:LEU:N	2.34	0.42
1:B:237:MET:C	1:B:238:LEU:HD23	2.44	0.42
1:B:341:LEU:O	1:B:344:ALA:N	2.51	0.42
1:B:338:THR:HG23	1:B:339:GLY:O	2.20	0.42
1:B:352:TYR:N	1:B:352:TYR:CD1	2.82	0.42
1:A:265:ASP:O	1:A:266:ALA:C	2.61	0.42
1:B:113:LEU:HA	1:B:113:LEU:HD12	1.52	0.42
1:A:375:CYS:C	1:A:377:LEU:H	2.27	0.41
1:A:223:ASP:O	1:A:224:LYS:C	2.63	0.41
1:B:70:MET:HE2	1:B:145:HIS:NE2	2.35	0.41
1:B:387:VAL:CG2	1:B:388:SER:H	2.23	0.41
1:B:229:PHE:HB2	3:B:606:HOH:O	2.20	0.41
1:A:69:LYS:HG2	1:A:132:PHE:CE1	2.55	0.41
1:A:67:GLN:O	1:A:68:ARG:C	2.63	0.41
1:A:96:ASN:HD22	1:A:96:ASN:C	2.29	0.41
1:A:138:ILE:HG12	1:A:141:MET:HE2	2.03	0.41
1:A:299:TYR:CE1	1:A:362:VAL:HG13	2.55	0.41
1:A:341:LEU:O	1:A:342:LEU:C	2.64	0.41
1:B:268:HIS:CD2	1:B:269:MET:N	2.89	0.41
1:A:118:HIS:HB3	1:B:118:HIS:CD2	2.56	0.40
1:B:60:ASP:OD1	1:B:60:ASP:N	2.52	0.40
1:B:161:THR:O	1:B:162:ALA:C	2.62	0.40
1:A:74:ILE:HA	1:A:142:VAL:HG22	2.02	0.40
1:A:102:ALA:HA	1:A:186:VAL:O	2.21	0.40
1:A:248:LYS:O	1:A:248:LYS:CG	2.65	0.40
1:B:19:THR:HG22	1:B:21:GLU:H	1.87	0.40
1:A:298:GLY:HA3	1:A:390:MET:HG3	2.03	0.40
1:B:78:ILE:HD11	1:B:145:HIS:CB	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HG21	1:B:111:LEU:CD1	2.49	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	407/443 (92%)	374 (92%)	28 (7%)	5 (1%)	10	27
1	B	408/443 (92%)	377 (92%)	29 (7%)	2 (0%)	24	48
All	All	815/886 (92%)	751 (92%)	57 (7%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	ARG
1	A	304	GLY
1	A	306	SER
1	A	375	CYS
1	B	304	GLY
1	B	194	SER
1	A	68	ARG

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	305/334 (91%)	268 (88%)	37 (12%)	5	12
1	B	306/334 (92%)	278 (91%)	28 (9%)	8	22
All	All	611/668 (92%)	546 (89%)	65 (11%)	6	17

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	SER
1	A	65	LYS
1	A	79	VAL
1	A	90	LEU
1	A	91	GLU
1	A	96	ASN
1	A	113	LEU
1	A	121	LEU
1	A	122	MET
1	A	137	THR
1	A	141	MET
1	A	153	ARG
1	A	186	VAL
1	A	197	LEU
1	A	208	LEU
1	A	214	ASN
1	A	216	GLN
1	A	231	LEU
1	A	238	LEU
1	A	252	LYS
1	A	275	ASN
1	A	281	LEU
1	A	288	ARG
1	A	293	GLU
1	A	301	ASN
1	A	327	SER
1	A	337	MET
1	A	338	THR
1	A	341	LEU
1	A	342	LEU
1	A	364	PRO
1	A	370	ASN
1	A	376	ASP
1	A	385	ARG
1	A	388	SER

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Mol	Chain	Res	Type
1	A	391	GLU
1	A	410	LYS
1	B	19	THR
1	B	43	SER
1	B	59	GLU
1	B	60	ASP
1	B	65	LYS
1	B	95	GLU
1	B	99	ARG
1	B	113	LEU
1	B	141	MET
1	B	186	VAL
1	B	197	LEU
1	B	206	ARG
1	B	208	LEU
1	B	216	GLN
1	B	221	PRO
1	B	238	LEU
1	B	275	ASN
1	B	281	LEU
1	B	301	ASN
1	B	324	GLU
1	B	327	SER
1	B	338	THR
1	B	375	CYS
1	B	383	GLU
1	B	385	ARG
1	B	391	GLU
1	B	406	SER
1	B	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	118	HIS
1	A	123	ASN
1	A	216	GLN
1	A	268	HIS
1	A	275	ASN
1	A	285	ASN
1	A	301	ASN

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Mol	Chain	Res	Type
1	A	382	HIS
1	B	18	ASN
1	B	118	HIS
1	B	123	ASN
1	B	214	ASN
1	B	268	HIS
1	B	301	ASN
1	B	367	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	A1EWE	A	501	-	48,49,49	2.24	15 (31%)	57,82,82	2.77	25 (43%)
2	A1EWE	B	501	-	48,49,49	2.00	10 (20%)	57,82,82	2.25	16 (28%)

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	A1EWE	A	501	-	-	7/20/78/78	0/1/7/7
2	A1EWE	B	501	-	-	6/20/78/78	0/1/7/7

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1EWE	C6-C7	6.70	1.44	1.35
2	A	501	A1EWE	C41-S40	-5.59	1.63	1.74
2	A	501	A1EWE	C6-C7	5.37	1.43	1.35
2	B	501	A1EWE	C4-C5	-5.24	1.46	1.53
2	A	501	A1EWE	C27-C22	-5.22	1.32	1.39
2	A	501	A1EWE	C24-N28	-5.00	1.34	1.43
2	A	501	A1EWE	C13-C8	4.19	1.61	1.54
2	B	501	A1EWE	O19-C5	-4.11	1.15	1.22
2	B	501	A1EWE	C42-C41	3.90	1.47	1.41
2	A	501	A1EWE	C43-C42	-3.81	1.33	1.39
2	B	501	A1EWE	C41-S40	-3.53	1.67	1.74
2	B	501	A1EWE	C24-N28	-3.50	1.37	1.43
2	A	501	A1EWE	C18-C4	3.28	1.59	1.54
2	B	501	A1EWE	C6-S40	-3.02	1.68	1.74
2	A	501	A1EWE	C42-C7	3.00	1.53	1.45
2	A	501	A1EWE	C11-C12	-2.94	1.47	1.53
2	A	501	A1EWE	C3-C4	2.74	1.61	1.54
2	B	501	A1EWE	C4-C9	-2.70	1.52	1.56
2	B	501	A1EWE	C22-C23	2.59	1.45	1.41
2	A	501	A1EWE	C43-C44	-2.49	1.35	1.39
2	A	501	A1EWE	O31-C23	-2.43	1.31	1.36
2	A	501	A1EWE	C14-C15	-2.39	1.49	1.53
2	B	501	A1EWE	C26-C25	-2.29	1.35	1.39
2	A	501	A1EWE	C11-C10	2.24	1.57	1.52
2	A	501	A1EWE	C46-C41	-2.21	1.36	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1EWE	C11-C12-C13	-9.21	100.72	107.92
2	A	501	A1EWE	C41-S40-C6	7.54	99.04	91.02
2	B	501	A1EWE	C3-C2-C1	-6.07	97.70	111.25
2	B	501	A1EWE	C11-C12-C13	-5.97	103.25	107.92
2	A	501	A1EWE	C23-C22-C21	5.94	126.50	119.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	A1EWE	C18-C4-C3	5.80	115.13	107.62
2	A	501	A1EWE	C27-C26-C25	5.69	126.19	120.50
2	B	501	A1EWE	O32-C21-C22	-4.62	110.95	121.97
2	B	501	A1EWE	C41-C42-C7	-4.50	106.26	111.50
2	A	501	A1EWE	C50-C47-C44	4.41	120.75	110.35
2	A	501	A1EWE	O20-C1-N28	4.24	131.24	123.64
2	A	501	A1EWE	C48-C47-C44	-3.99	100.94	110.35
2	B	501	A1EWE	C14-C8-C13	3.82	108.44	101.94
2	B	501	A1EWE	C23-C22-C21	3.58	123.86	119.86
2	B	501	A1EWE	C42-C41-S40	3.49	116.34	112.24
2	B	501	A1EWE	O33-C21-C22	3.40	124.95	115.28
2	A	501	A1EWE	C43-C42-C41	-3.35	114.63	119.42
2	A	501	A1EWE	C17-C15-C14	-3.35	110.21	115.17
2	A	501	A1EWE	C7-C6-S40	-3.23	107.39	114.17
2	A	501	A1EWE	C27-C22-C23	-3.16	115.69	118.76
2	A	501	A1EWE	O33-C21-C22	2.99	123.77	115.28
2	A	501	A1EWE	C18-C4-C9	2.82	120.34	114.22
2	A	501	A1EWE	C48-C47-C49	2.82	116.73	108.36
2	A	501	A1EWE	C15-O16-C10	-2.79	93.42	105.83
2	B	501	A1EWE	C2-C3-C4	2.75	120.88	115.58
2	B	501	A1EWE	C46-C41-C42	-2.64	118.70	121.47
2	A	501	A1EWE	O16-C15-C17	2.61	112.88	108.05
2	A	501	A1EWE	O16-C10-C11	2.59	109.39	102.98
2	A	501	A1EWE	O20-C1-C2	-2.40	117.67	122.02
2	B	501	A1EWE	C49-C47-C44	-2.38	104.73	110.35
2	A	501	A1EWE	C46-C41-C42	2.28	123.86	121.47
2	B	501	A1EWE	O31-C23-C22	2.26	125.14	121.11
2	A	501	A1EWE	C22-C23-C24	2.23	124.06	119.98
2	A	501	A1EWE	C14-C8-C13	2.22	105.72	101.94
2	B	501	A1EWE	C8-C13-C12	-2.17	93.23	102.49
2	A	501	A1EWE	O32-C21-C22	-2.16	116.82	121.97
2	B	501	A1EWE	O30-C25-C26	2.15	125.12	119.36
2	B	501	A1EWE	C18-C4-C5	-2.11	102.08	107.01
2	A	501	A1EWE	C17-C15-C12	-2.09	110.71	115.18
2	A	501	A1EWE	C18-C4-C5	-2.05	102.21	107.01
2	A	501	A1EWE	C2-C1-N28	-2.03	111.05	114.59

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1EWE	C45-C44-C47-C48

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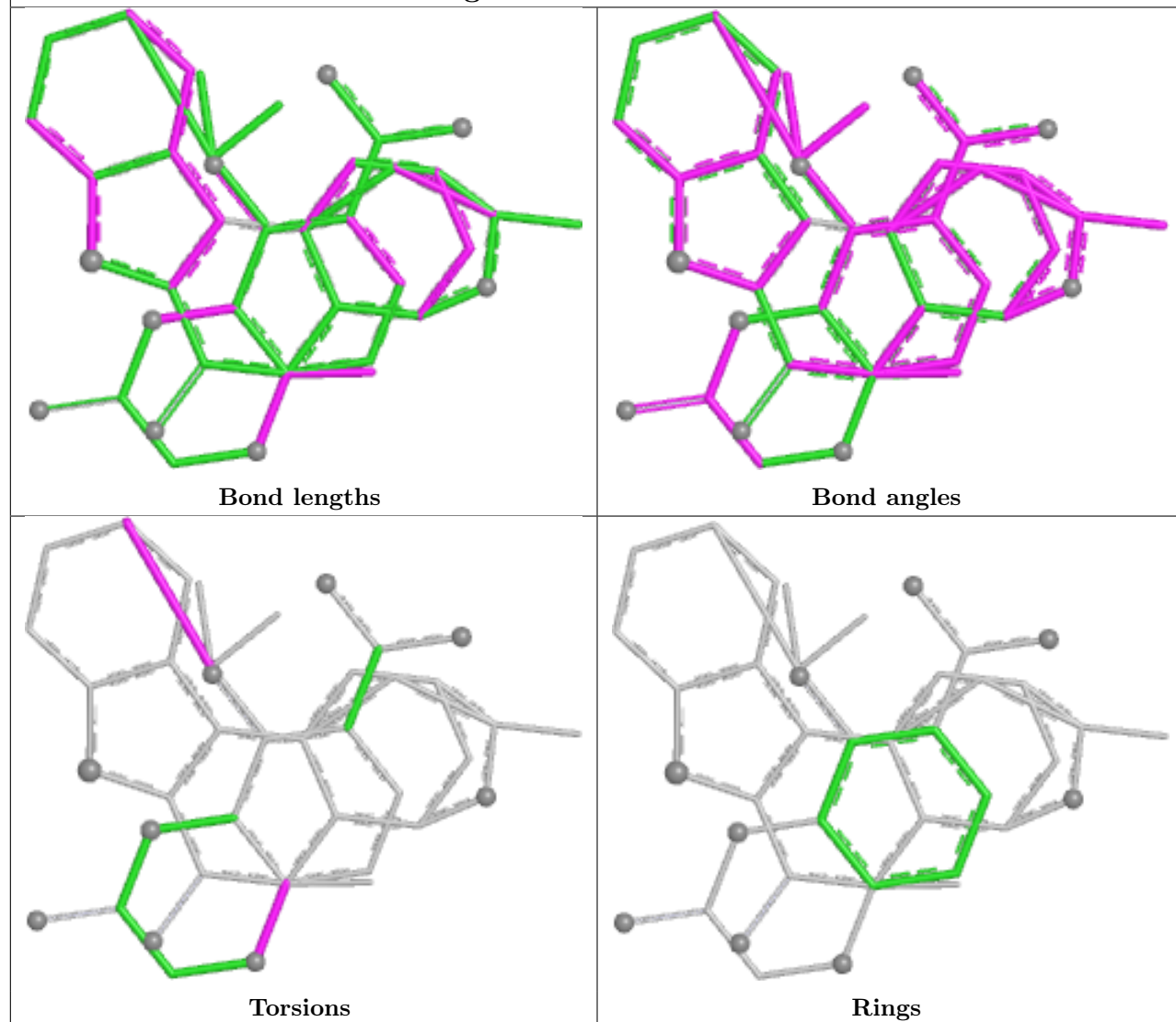
Mol	Chain	Res	Type	Atoms
2	A	501	A1EWE	C2-C3-C4-C18
2	B	501	A1EWE	C43-C44-C47-C49
2	A	501	A1EWE	C2-C3-C4-C5
2	B	501	A1EWE	C45-C44-C47-C49
2	B	501	A1EWE	C43-C44-C47-C48
2	B	501	A1EWE	C45-C44-C47-C48
2	A	501	A1EWE	C45-C44-C47-C49
2	A	501	A1EWE	C43-C44-C47-C50
2	B	501	A1EWE	C43-C44-C47-C50
2	A	501	A1EWE	C45-C44-C47-C50
2	A	501	A1EWE	C43-C44-C47-C49
2	B	501	A1EWE	O32-C21-C22-C23

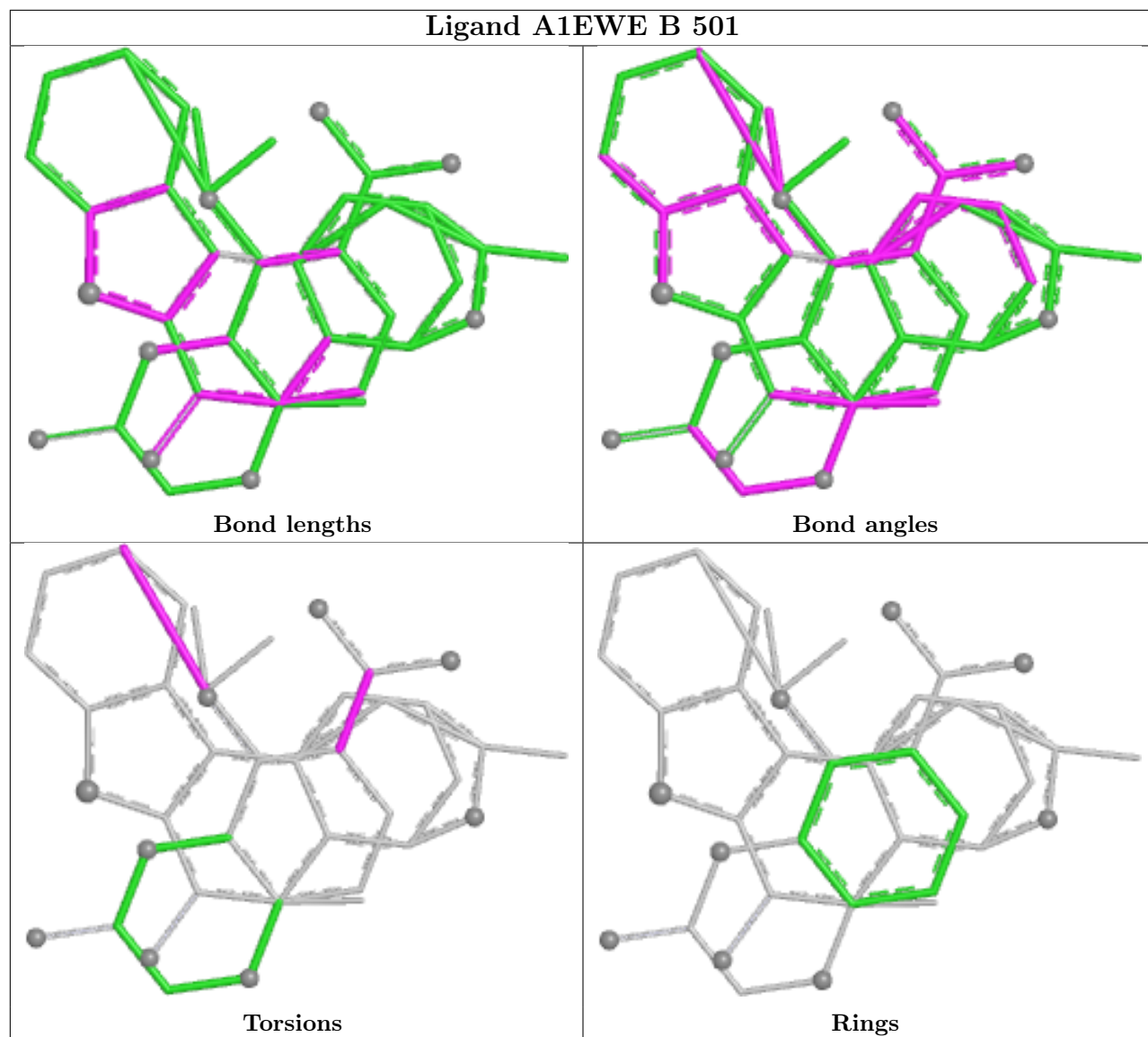
There are no ring outliers.

No monomer is involved in short contacts.

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 A1EWE A 501





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	409/443 (92%)	0.25	12 (2%) 53 50	34, 54, 89, 113	0
1	B	410/443 (92%)	0.47	18 (4%) 39 35	36, 56, 85, 116	0
All	All	819/886 (92%)	0.36	30 (3%) 45 41	34, 55, 88, 116	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	VAL	8.4
1	B	361	ALA	6.9
1	B	101	GLY	6.6
1	B	257	LEU	4.7
1	B	318	VAL	4.5
1	A	199	VAL	4.4
1	B	183	ASP	4.3
1	B	186	VAL	3.9
1	A	331	VAL	3.3
1	B	102	ALA	3.3
1	A	361	ALA	3.2
1	A	300	VAL	3.1
1	A	60	ASP	2.9
1	A	362	VAL	2.8
1	B	409	PHE	2.8
1	A	238	LEU	2.7
1	B	122	MET	2.7
1	B	330	LEU	2.7
1	A	253	ILE	2.5
1	B	284	ALA	2.5
1	B	348	VAL	2.4
1	B	322	PHE	2.3
1	A	411	LYS	2.3
1	B	352	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	MET	2.1
1	B	387	VAL	2.1
1	A	121	LEU	2.1
1	B	287	LEU	2.1
1	A	38	ASP	2.0
1	B	173	ALA	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](#)

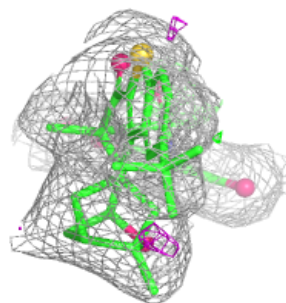
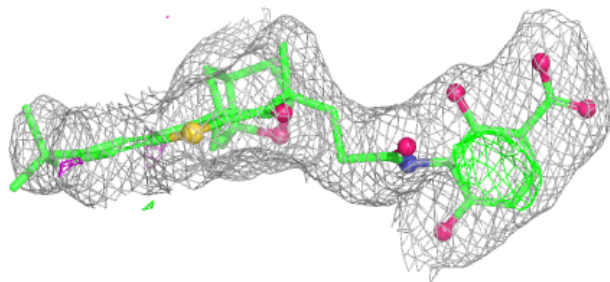
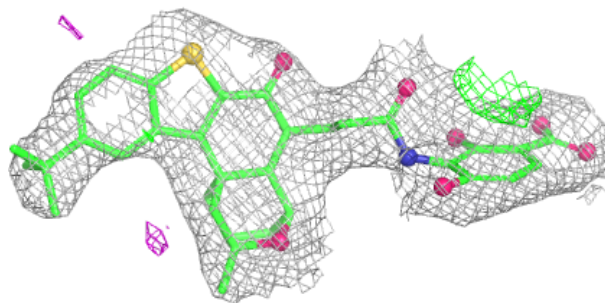
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1EWE	B	501	43/43	0.93	0.09	32,47,83,95	0
2	A1EWE	A	501	43/43	0.94	0.08	32,47,69,74	0

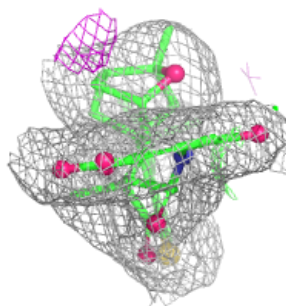
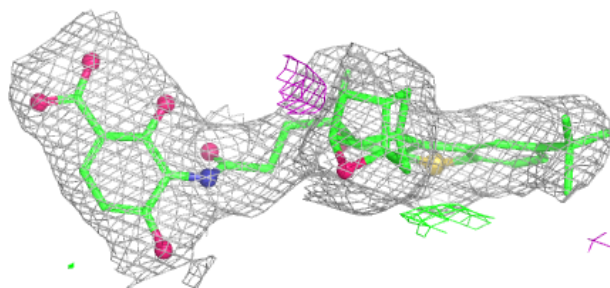
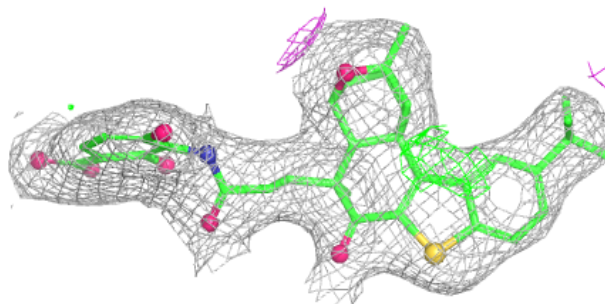
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1EWE B 501:

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

**Electron density around A1EWE A 501:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.