



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2026 – 06:57 AM JST

PDB ID : 9K99 / pdb_00009k99
Title : Crystal structure of Setaria viridis SPS complexed with Aclonifen (surface polar residue mutant)
Authors : Xiao, H.; Li, M.; Yang, G.-F.
Deposited on : 2024-10-26
Resolution : 2.65 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	:	1.8.5 (274361), CSD as541be (2020)
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

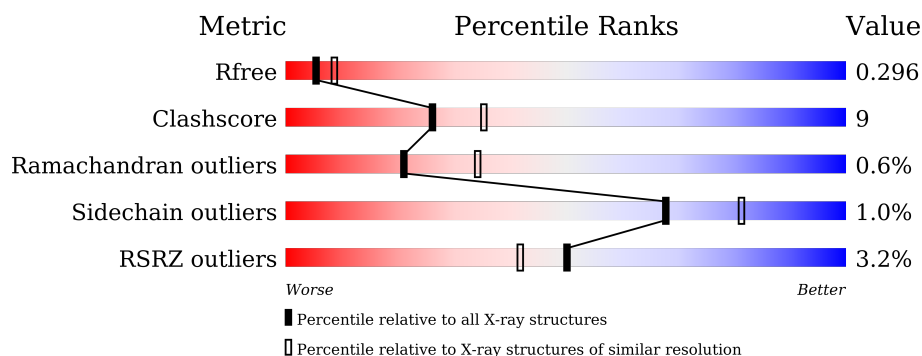
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	324	<div> <div>4%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	B	324	<div> <div>2%</div> <div>73%</div> <div>20%</div> <div>7%</div> </div>
1	C	324	<div> <div>2%</div> <div>66%</div> <div>14%</div> <div>20%</div> </div>
1	D	324	<div> <div>2%</div> <div>58%</div> <div>15%</div> <div>26%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8573 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 Solanesyl diphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2396	1522	400	467	7			
1	B	302	Total	C	N	O	S	0	0	0
			2315	1469	389	450	7			
1	C	259	Total	C	N	O	S	0	0	0
			1988	1263	331	387	7			
1	D	240	Total	C	N	O	S	0	0	0
			1831	1162	304	357	8			

There are 60 discrepancies between the modelled and reference sequences:

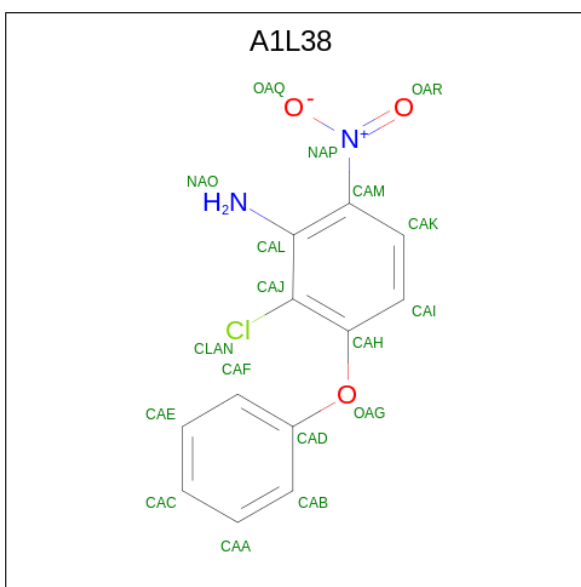
Chain	Residue	Modelled	Actual	Comment	Reference
A	114	ALA	SER	engineered mutation	UNP A0A4U6VI49
A	169	LEU	SER	engineered mutation	UNP A0A4U6VI49
A	303	ALA	GLU	engineered mutation	UNP A0A4U6VI49
A	304	ALA	GLN	engineered mutation	UNP A0A4U6VI49
A	358	GLN	GLU	engineered mutation	UNP A0A4U6VI49
A	371	ASN	ASP	engineered mutation	UNP A0A4U6VI49
A	375	THR	ALA	engineered mutation	UNP A0A4U6VI49
A	378	GLU	ASP	engineered mutation	UNP A0A4U6VI49
A	387	LYS	ARG	engineered mutation	UNP A0A4U6VI49
A	398	GLU	ASP	engineered mutation	UNP A0A4U6VI49
A	399	ILE	LEU	engineered mutation	UNP A0A4U6VI49
A	403	SER	ASN	engineered mutation	UNP A0A4U6VI49
A	411	GLU	ASP	engineered mutation	UNP A0A4U6VI49
A	417	ALA	GLU	engineered mutation	UNP A0A4U6VI49
A	418	ALA	LYS	engineered mutation	UNP A0A4U6VI49
B	114	ALA	SER	engineered mutation	UNP A0A4U6VI49
B	169	LEU	SER	engineered mutation	UNP A0A4U6VI49
B	303	ALA	GLU	engineered mutation	UNP A0A4U6VI49
B	304	ALA	GLN	engineered mutation	UNP A0A4U6VI49
B	358	GLN	GLU	engineered mutation	UNP A0A4U6VI49
B	371	ASN	ASP	engineered mutation	UNP A0A4U6VI49

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	THR	ALA	engineered mutation	UNP A0A4U6VI49
B	378	GLU	ASP	engineered mutation	UNP A0A4U6VI49
B	387	LYS	ARG	engineered mutation	UNP A0A4U6VI49
B	398	GLU	ASP	engineered mutation	UNP A0A4U6VI49
B	399	ILE	LEU	engineered mutation	UNP A0A4U6VI49
B	403	SER	ASN	engineered mutation	UNP A0A4U6VI49
B	411	GLU	ASP	engineered mutation	UNP A0A4U6VI49
B	417	ALA	GLU	engineered mutation	UNP A0A4U6VI49
B	418	ALA	LYS	engineered mutation	UNP A0A4U6VI49
C	114	ALA	SER	engineered mutation	UNP A0A4U6VI49
C	169	LEU	SER	engineered mutation	UNP A0A4U6VI49
C	303	ALA	GLU	engineered mutation	UNP A0A4U6VI49
C	304	ALA	GLN	engineered mutation	UNP A0A4U6VI49
C	358	GLN	GLU	engineered mutation	UNP A0A4U6VI49
C	371	ASN	ASP	engineered mutation	UNP A0A4U6VI49
C	375	THR	ALA	engineered mutation	UNP A0A4U6VI49
C	378	GLU	ASP	engineered mutation	UNP A0A4U6VI49
C	387	LYS	ARG	engineered mutation	UNP A0A4U6VI49
C	398	GLU	ASP	engineered mutation	UNP A0A4U6VI49
C	399	ILE	LEU	engineered mutation	UNP A0A4U6VI49
C	403	SER	ASN	engineered mutation	UNP A0A4U6VI49
C	411	GLU	ASP	engineered mutation	UNP A0A4U6VI49
C	417	ALA	GLU	engineered mutation	UNP A0A4U6VI49
C	418	ALA	LYS	engineered mutation	UNP A0A4U6VI49
D	114	ALA	SER	engineered mutation	UNP A0A4U6VI49
D	169	LEU	SER	engineered mutation	UNP A0A4U6VI49
D	303	ALA	GLU	engineered mutation	UNP A0A4U6VI49
D	304	ALA	GLN	engineered mutation	UNP A0A4U6VI49
D	358	GLN	GLU	engineered mutation	UNP A0A4U6VI49
D	371	ASN	ASP	engineered mutation	UNP A0A4U6VI49
D	375	THR	ALA	engineered mutation	UNP A0A4U6VI49
D	378	GLU	ASP	engineered mutation	UNP A0A4U6VI49
D	387	LYS	ARG	engineered mutation	UNP A0A4U6VI49
D	398	GLU	ASP	engineered mutation	UNP A0A4U6VI49
D	399	ILE	LEU	engineered mutation	UNP A0A4U6VI49
D	403	SER	ASN	engineered mutation	UNP A0A4U6VI49
D	411	GLU	ASP	engineered mutation	UNP A0A4U6VI49
D	417	ALA	GLU	engineered mutation	UNP A0A4U6VI49
D	418	ALA	LYS	engineered mutation	UNP A0A4U6VI49

- Molecule 2 is Acclonifen (CCD ID: A1L38) (formula: $C_{12}H_9ClN_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 18	C 12	Cl 1	N 2	O 3	0	0
2	D	1	Total 18	C 12	Cl 1	N 2	O 3	0	0

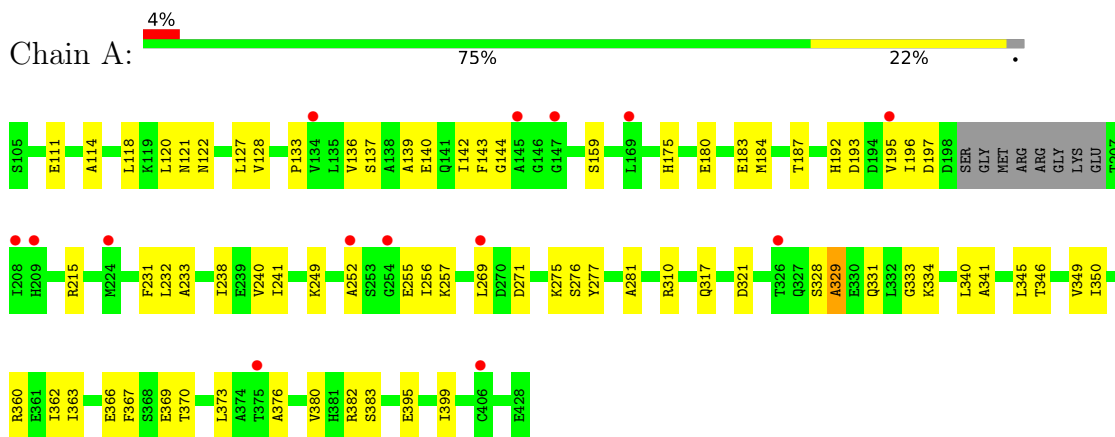
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

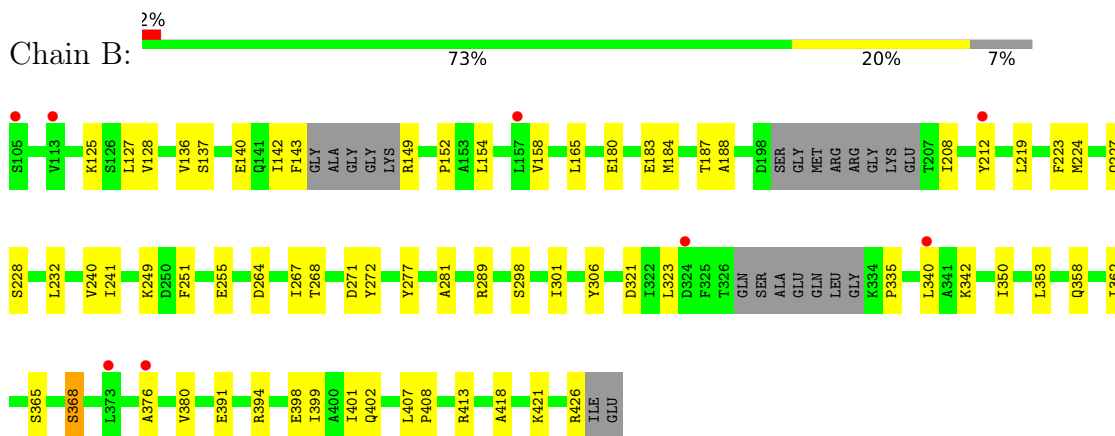
3 Residue-property plots [i](#)

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.

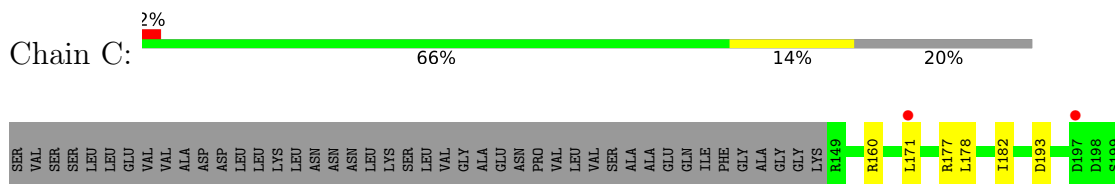
- Molecule 1: Solanesyl diphosphate synthase

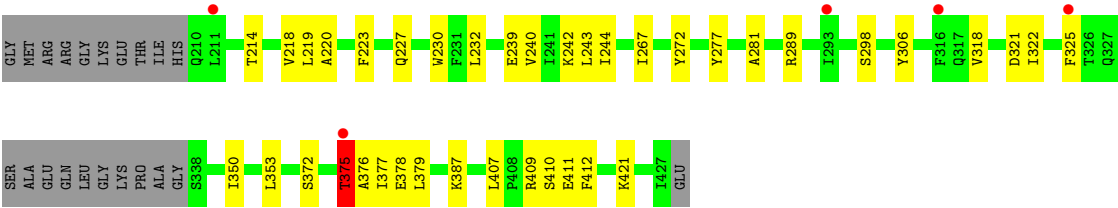


- Molecule 1: Solanesyl diphosphate synthase

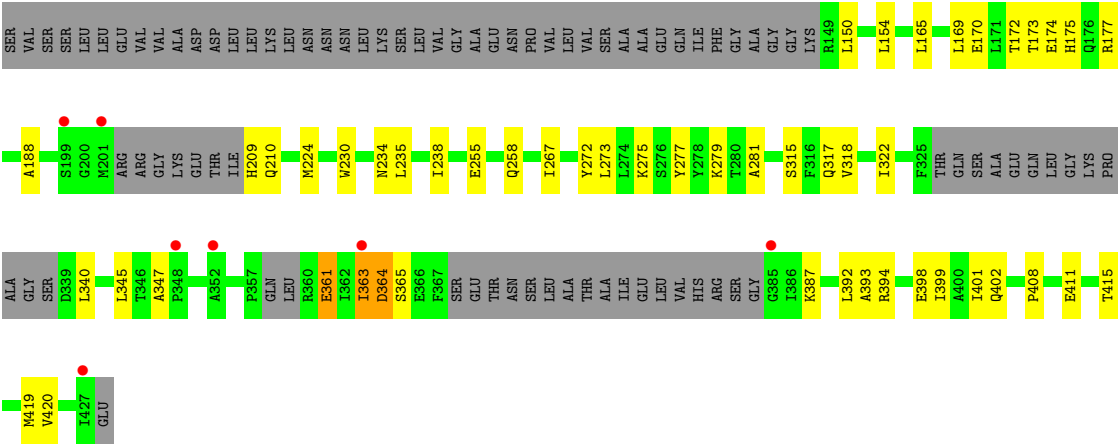


- Molecule 1: Solanesyl diphosphate synthase





● Molecule 1: Solanesyl diphosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.38Å 69.10Å 80.58Å 104.95° 112.43° 92.10°	Depositor
Resolution (Å)	42.55 – 2.65 42.55 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.0 (42.55-2.65) 98.0 (42.55-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.16_3549: ???)	Depositor
R, R_{free}	0.242 , 0.297 0.243 , 0.296	Depositor DCC
R_{free} test set	1792 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8573	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1L38

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	0.29	0/2428	0.51	0/3289
1	B	0.11	0/2344	0.33	1/3175 (0.0%)
1	C	0.27	0/2014	0.47	1/2726 (0.0%)
1	D	0.21	0/1852	0.43	1/2503 (0.0%)
All	All	0.23	0/8638	0.44	3/11693 (0.0%)

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	C	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	364	ASP	N-CA-C	-7.31	103.62	112.54
1	B	399	ILE	N-CA-C	-5.70	107.26	112.96
1	C	412	PHE	N-CA-CB	-5.66	101.80	110.01

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	360	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	409	ARG	Sidechain

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	2396	0	2409	47	0
1	B	2315	0	2333	42	0
1	C	1988	0	1990	33	0
1	D	1831	0	1824	44	0
2	C	18	0	0	1	0
2	D	18	0	0	1	0
3	A	4	0	0	1	0
3	B	2	0	0	1	0
3	C	1	0	0	0	0
All	All	8573	0	8556	161	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 9.

All (161) 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:D:150:LEU:O	1:D:154:LEU:HD13	1.55	1.07
1:A:137:SER:HA	1:A:140:GLU:HB2	1.64	0.77
1:D:150:LEU:O	1:D:154:LEU:CD1	2.35	0.75
1:A:111:GLU:HA	1:A:114:ALA:HB2	1.72	0.71
1:C:375:THR:HG22	1:C:379:LEU:HD11	1.74	0.70
1:B:298:SER:HB3	1:B:301:ILE:HD12	1.74	0.69
1:B:184:MET:HG3	1:B:228:SER:HB3	1.75	0.67
1:B:398:GLU:HA	1:B:401:ILE:HG12	1.77	0.67
1:A:139:ALA:HA	1:A:142:ILE:HG12	1.77	0.66
1:B:188:ALA:HB2	1:B:224:MET:HB2	1.77	0.65
1:D:150:LEU:C	1:D:154:LEU:HD13	2.22	0.65
1:D:361:GLU:HA	1:D:364:ASP:HB2	1.80	0.63
1:B:277:TYR:HA	1:B:281:ALA:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD12	1:A:238:ILE:H	1.63	0.62
1:B:268:THR:HG1	1:B:271:ASP:H	1.45	0.62
1:A:256:ILE:HG13	1:C:219:LEU:HD21	1.82	0.61
1:A:271:ASP:O	1:A:275:LYS:HG3	2.00	0.61
1:C:350:ILE:HA	1:C:353:LEU:HD12	1.82	0.61
1:A:128:VAL:CG2	1:A:136:VAL:HG12	2.32	0.60
1:A:120:LEU:HD12	1:A:180:GLU:HG3	1.83	0.60
1:A:340:LEU:HD13	1:A:349:VAL:HG21	1.84	0.60
1:B:289:ARG:HD2	1:B:306:TYR:HB2	1.83	0.59
1:B:407:LEU:O	1:B:413:ARG:NH1	2.36	0.59
1:D:340:LEU:HD21	1:D:363:ILE:HG12	1.84	0.58
1:B:391:GLU:HA	1:B:394:ARG:HG2	1.86	0.58
1:A:127:LEU:CD2	1:A:128:VAL:HG13	2.34	0.58
1:B:264:ASP:O	1:B:267:ILE:HG13	2.03	0.57
1:A:184:MET:HE1	1:A:231:PHE:HD2	1.70	0.57
1:A:133:PRO:O	1:A:136:VAL:HG22	2.05	0.57
1:D:277:TYR:HA	1:D:281:ALA:HB3	1.87	0.57
2:D:501:A1L38:NAO	2:D:501:A1L38:OAR	2.38	0.57
1:C:375:THR:O	1:C:379:LEU:HD12	2.04	0.56
1:C:375:THR:O	1:C:376:ALA:C	2.47	0.56
1:D:345:LEU:O	1:D:345:LEU:HD12	2.06	0.56
1:D:340:LEU:CD2	1:D:363:ILE:HG12	2.36	0.55
1:D:394:ARG:O	1:D:398:GLU:HG2	2.06	0.55
1:D:165:LEU:HD13	1:D:408:PRO:HD3	1.89	0.55
1:D:209:HIS:CG	1:D:210:GLN:H	2.25	0.55
1:D:267:ILE:HG21	1:D:345:LEU:CD1	2.37	0.55
1:B:342:LYS:NZ	3:B:501:HOH:O	2.40	0.54
2:C:501:A1L38:NAO	2:C:501:A1L38:OAQ	2.40	0.54
1:C:325:PHE:HZ	1:C:377:ILE:HA	1.71	0.54
1:C:375:THR:O	1:C:378:GLU:HG2	2.08	0.54
1:A:277:TYR:HA	1:A:281:ALA:HB3	1.88	0.54
1:B:323:LEU:HD21	1:B:426:ARG:HG3	1.88	0.54
1:A:118:LEU:HD13	1:A:118:LEU:C	2.32	0.53
1:B:232:LEU:HD21	1:B:241:ILE:HA	1.91	0.53
1:C:243:LEU:HD11	1:C:289:ARG:HD3	1.90	0.53
1:C:277:TYR:HA	1:C:281:ALA:HB3	1.90	0.52
1:B:418:ALA:O	1:B:421:LYS:HG3	2.10	0.52
1:D:318:VAL:O	1:D:322:ILE:HG13	2.09	0.52
1:D:150:LEU:CD1	1:D:154:LEU:HD11	2.39	0.52
1:A:128:VAL:HG23	1:A:136:VAL:HG12	1.92	0.52
1:A:276:SER:HB3	1:A:317:GLN:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:PHE:HE2	1:A:187:THR:HG21	1.75	0.51
1:A:257:LYS:HD3	1:A:275:LYS:HG2	1.91	0.51
1:C:220:ALA:HA	1:C:223:PHE:CE2	2.45	0.51
1:D:230:TRP:O	1:D:234:ASN:ND2	2.37	0.51
1:B:142:ILE:HG21	1:B:187:THR:HG23	1.92	0.51
1:C:239:GLU:HG3	1:C:242:LYS:HE3	1.91	0.51
1:C:177:ARG:CZ	1:D:177:ARG:HD2	2.41	0.51
1:C:223:PHE:O	1:C:227:GLN:HG2	2.10	0.51
1:B:154:LEU:O	1:B:158:VAL:HG12	2.11	0.51
1:C:160:ARG:HG3	1:C:171:LEU:HD11	1.92	0.51
1:B:350:ILE:HA	1:B:353:LEU:HD23	1.93	0.51
1:D:267:ILE:HG21	1:D:345:LEU:HD11	1.92	0.51
1:C:240:VAL:O	1:C:244:ILE:HG12	2.11	0.50
1:D:172:THR:HG22	1:D:175:HIS:ND1	2.26	0.50
1:A:193:ASP:O	1:A:197:ASP:HB2	2.12	0.50
1:C:376:ALA:HA	1:C:379:LEU:HD13	1.93	0.50
1:D:273:LEU:HD21	1:D:392:LEU:HD21	1.93	0.49
1:D:150:LEU:HG	1:D:154:LEU:CD1	2.43	0.48
1:B:376:ALA:O	1:B:380:VAL:HG22	2.14	0.48
1:D:258:GLN:HG3	1:D:275:LYS:NZ	2.29	0.48
1:A:380:VAL:O	1:A:383:SER:OG	2.29	0.47
1:A:252:ALA:HA	1:A:255:GLU:HB2	1.97	0.47
1:D:173:THR:O	1:D:177:ARG:HG2	2.14	0.47
1:B:180:GLU:O	1:B:184:MET:HG2	2.15	0.47
1:B:223:PHE:HD1	1:B:224:MET:HE2	1.80	0.46
1:A:310:ARG:NH1	3:A:503:HOH:O	2.48	0.46
1:D:411:GLU:O	1:D:415:THR:OG1	2.31	0.46
1:B:128:VAL:HG21	1:B:136:VAL:HA	1.98	0.46
1:C:160:ARG:CG	1:C:171:LEU:HD11	2.46	0.46
1:C:387:LYS:HB3	1:C:387:LYS:HE3	1.74	0.46
1:B:137:SER:OG	1:B:212:TYR:OH	2.29	0.46
1:B:251:PHE:O	1:B:255:GLU:HG2	2.16	0.46
1:A:192:HIS:O	1:A:196:ILE:HG13	2.15	0.46
1:D:419:MET:HE2	1:D:419:MET:HB2	1.87	0.46
1:A:118:LEU:HD13	1:A:118:LEU:O	2.15	0.46
1:B:232:LEU:HD11	1:B:240:VAL:HG12	1.98	0.46
1:D:363:ILE:HD12	1:D:363:ILE:HA	1.83	0.46
1:B:125:LYS:NZ	1:B:140:GLU:HA	2.31	0.46
1:A:334:LYS:H	1:A:334:LYS:HG2	1.61	0.45
1:D:272:TYR:CE2	1:D:347:ALA:HB2	2.51	0.45
1:A:232:LEU:HD11	1:A:240:VAL:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:HD11	1:A:363:ILE:HG21	1.98	0.45
1:B:232:LEU:HG	1:B:241:ILE:HG12	1.99	0.45
1:A:127:LEU:HD23	1:A:128:VAL:HG13	1.97	0.45
1:A:317:GLN:HE21	1:A:321:ASP:CG	2.24	0.45
1:A:366:GLU:OE2	1:D:209:HIS:ND1	2.36	0.45
1:B:184:MET:HE1	1:B:227:GLN:HG2	1.98	0.45
1:A:328:SER:H	1:A:331:GLN:HE21	1.65	0.45
1:A:183:GLU:O	1:A:187:THR:HG23	2.16	0.45
1:D:315:SER:HA	1:D:318:VAL:HG22	1.98	0.45
1:D:398:GLU:HA	1:D:401:ILE:HD12	1.98	0.45
1:A:232:LEU:HD21	1:A:241:ILE:HA	1.99	0.45
1:D:340:LEU:HD23	1:D:340:LEU:O	2.16	0.45
1:A:215:ARG:NH1	1:C:193:ASP:OD2	2.50	0.44
1:C:289:ARG:HB2	1:C:306:TYR:HB2	1.98	0.44
1:B:401:ILE:HG13	1:B:402:GLN:N	2.33	0.44
1:C:375:THR:O	1:C:377:ILE:N	2.51	0.44
1:C:375:THR:C	1:C:379:LEU:HD12	2.43	0.44
1:C:421:LYS:HD3	1:C:421:LYS:HA	1.83	0.44
1:D:401:ILE:HD11	1:D:420:VAL:HG11	2.00	0.43
1:B:208:ILE:HG13	1:B:212:TYR:HD2	1.82	0.43
1:A:118:LEU:HD11	1:A:122:ASN:HD21	1.82	0.43
1:B:358:GLN:O	1:B:362:ILE:HG13	2.18	0.43
1:B:362:ILE:HA	1:B:365:SER:HB3	2.01	0.43
1:C:272:TYR:OH	1:C:321:ASP:OD2	2.31	0.43
1:A:329:ALA:O	1:A:333:GLY:N	2.51	0.43
1:A:341:ALA:HA	1:A:367:PHE:CE2	2.53	0.43
1:A:192:HIS:O	1:A:195:VAL:HG22	2.19	0.42
1:A:233:ALA:HA	1:A:241:ILE:HD11	2.00	0.42
1:B:272:TYR:OH	1:B:321:ASP:OD2	2.21	0.42
1:D:363:ILE:C	1:D:365:SER:N	2.76	0.42
1:B:219:LEU:HD13	1:D:255:GLU:HB3	2.01	0.42
1:C:318:VAL:O	1:C:322:ILE:HG13	2.20	0.42
1:C:325:PHE:CZ	1:C:377:ILE:HA	2.52	0.42
1:A:249:LYS:HD3	1:C:230:TRP:CD2	2.54	0.42
1:A:120:LEU:CD1	1:A:180:GLU:HG3	2.49	0.42
1:B:137:SER:O	1:B:140:GLU:HG2	2.19	0.42
1:B:249:LYS:HZ3	1:D:230:TRP:CD1	2.38	0.42
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.92	0.42
1:D:279:LYS:HE3	1:D:317:GLN:NE2	2.35	0.42
1:C:214:THR:O	1:C:218:VAL:HG23	2.20	0.41
1:B:340:LEU:H	1:B:340:LEU:HD23	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ILE:HG23	1:C:350:ILE:HG12	2.02	0.41
1:D:238:ILE:HD12	1:D:238:ILE:N	2.35	0.41
1:D:387:LYS:HE2	1:D:387:LYS:HB3	1.86	0.41
1:A:159:SER:HB3	1:A:175:HIS:CD2	2.55	0.41
1:B:365:SER:OG	1:B:368:SER:N	2.45	0.41
1:B:152:PRO:HG3	1:B:183:GLU:HB2	2.02	0.41
1:C:232:LEU:HD11	1:C:240:VAL:HG12	2.02	0.41
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.82	0.41
1:A:346:THR:O	1:A:350:ILE:HG13	2.20	0.41
1:C:375:THR:O	1:C:378:GLU:N	2.53	0.41
1:D:399:ILE:HA	1:D:402:GLN:HG2	2.03	0.41
1:B:165:LEU:HD21	1:B:408:PRO:HG3	2.02	0.41
1:B:143:PHE:HA	1:B:149:ARG:HH22	1.85	0.41
1:A:121:ASN:ND2	1:A:144:GLY:H	2.18	0.41
1:B:127:LEU:HD11	1:B:184:MET:HE1	2.02	0.41
1:B:268:THR:O	1:B:350:ILE:HD13	2.20	0.41
1:D:258:GLN:NE2	1:D:275:LYS:HD3	2.35	0.41
1:D:318:VAL:HG21	1:D:393:ALA:HA	2.03	0.41
1:A:373:LEU:O	1:A:376:ALA:N	2.54	0.41
1:D:150:LEU:HG	1:D:154:LEU:HD13	2.02	0.40
1:D:174:GLU:HG2	1:D:235:LEU:HD22	2.03	0.40
1:A:395:GLU:O	1:A:399:ILE:HG12	2.21	0.40
1:C:178:LEU:O	1:C:182:ILE:HG12	2.20	0.40
1:D:188:ALA:HB2	1:D:224:MET:HB2	2.02	0.40
1:D:169:LEU:HD23	1:D:170:GLU:H	1.85	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	312/324 (96%)	292 (94%)	18 (6%)	2 (1%)	21 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	294/324 (91%)	279 (95%)	13 (4%)	2 (1%)	18	30
1	C	253/324 (78%)	243 (96%)	8 (3%)	2 (1%)	16	27
1	D	230/324 (71%)	220 (96%)	10 (4%)	0	100	100
All	All	1089/1296 (84%)	1034 (95%)	49 (4%)	6 (1%)	21	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	329	ALA
1	B	368	SER
1	C	298	SER
1	C	375	THR
1	A	382	ARG
1	B	335	PRO

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	255/268 (95%)	252 (99%)	3 (1%)	63	79
1	B	250/268 (93%)	250 (100%)	0	100	100
1	C	213/268 (80%)	209 (98%)	4 (2%)	50	71
1	D	194/268 (72%)	192 (99%)	2 (1%)	68	81
All	All	912/1072 (85%)	903 (99%)	9 (1%)	68	81

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	362	ILE
1	A	369	GLU
1	A	370	THR
1	C	372	SER
1	C	375	THR

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Mol	Chain	Res	Type
1	C	410	SER
1	C	411	GLU
1	D	361	GLU
1	D	363	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	122	ASN
1	A	132	ASN
1	A	176	GLN
1	A	186	HIS
1	A	327	GLN
1	B	132	ASN
1	B	141	GLN
1	B	246	GLN
1	B	354	GLN
1	C	317	GLN
1	C	405	GLN
1	D	246	GLN
1	D	405	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1L38	D	501	-	18,19,19	2.79	6 (33%)	19,26,26	1.27	2 (10%)
2	A1L38	C	501	-	18,19,19	2.79	5 (27%)	19,26,26	1.16	2 (10%)

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	A1L38	D	501	-	-	1/6/8/8	0/2/2/2
2	A1L38	C	501	-	-	1/6/8/8	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	A1L38	OAR-NAP	7.97	1.36	1.22
2	D	501	A1L38	OAR-NAP	7.83	1.36	1.22
2	D	501	A1L38	CAM-NAP	-7.05	1.32	1.45
2	C	501	A1L38	CAM-NAP	-7.03	1.32	1.45
2	D	501	A1L38	CAL-CAM	-2.83	1.38	1.42
2	C	501	A1L38	CAJ-CLAN	2.79	1.78	1.72
2	D	501	A1L38	CAJ-CLAN	2.75	1.78	1.72
2	C	501	A1L38	CAL-CAM	-2.71	1.39	1.42
2	D	501	A1L38	CAL-NAO	2.66	1.45	1.37
2	C	501	A1L38	CAL-NAO	2.65	1.45	1.37
2	D	501	A1L38	CAL-CAJ	-2.14	1.38	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	A1L38	CAK-CAM-NAP	3.92	120.66	116.47
2	C	501	A1L38	CAK-CAM-NAP	2.97	119.65	116.47
2	D	501	A1L38	CAM-CAL-NAO	-2.93	120.20	124.11
2	C	501	A1L38	CAM-CAL-NAO	-2.87	120.28	124.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	A1L38	CAJ-CAH-OAG-CAD
2	C	501	A1L38	CAJ-CAH-OAG-CAD

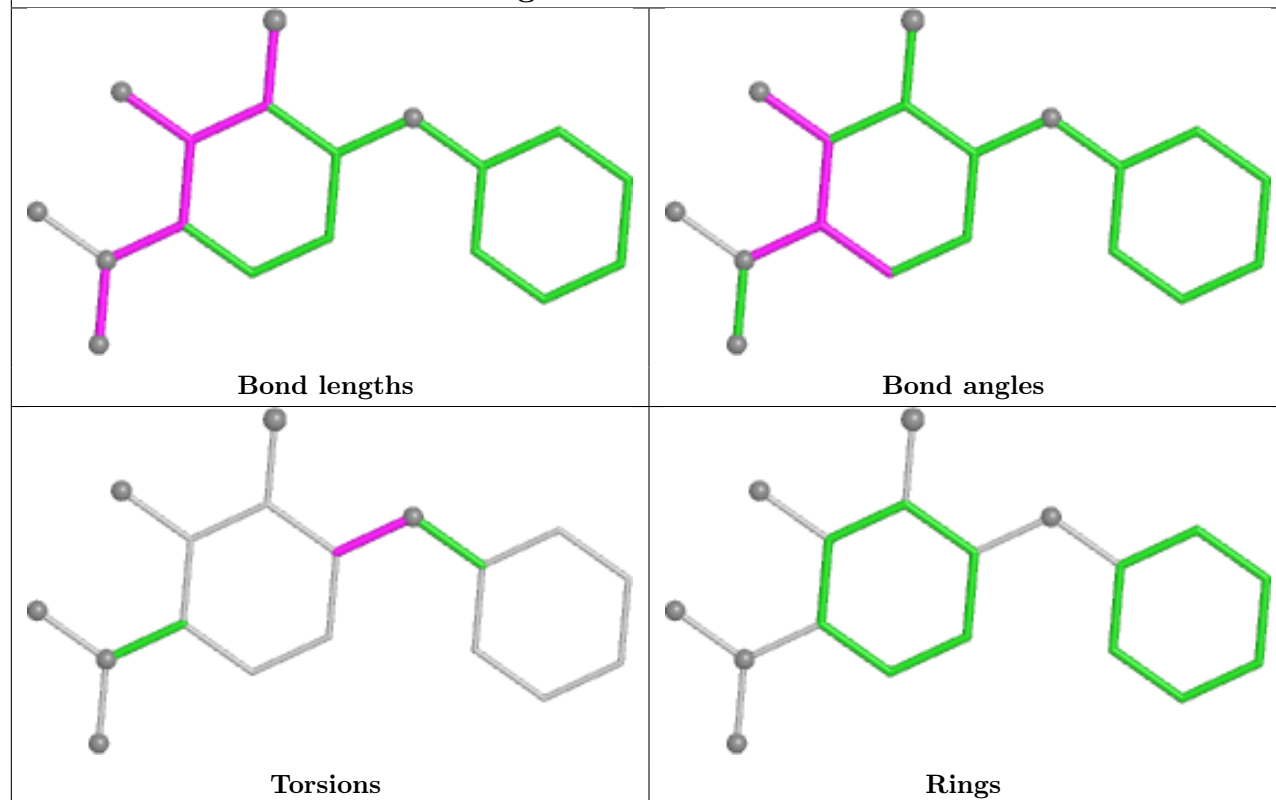
There are no ring outliers.

2 monomers are involved in 2 short contacts:

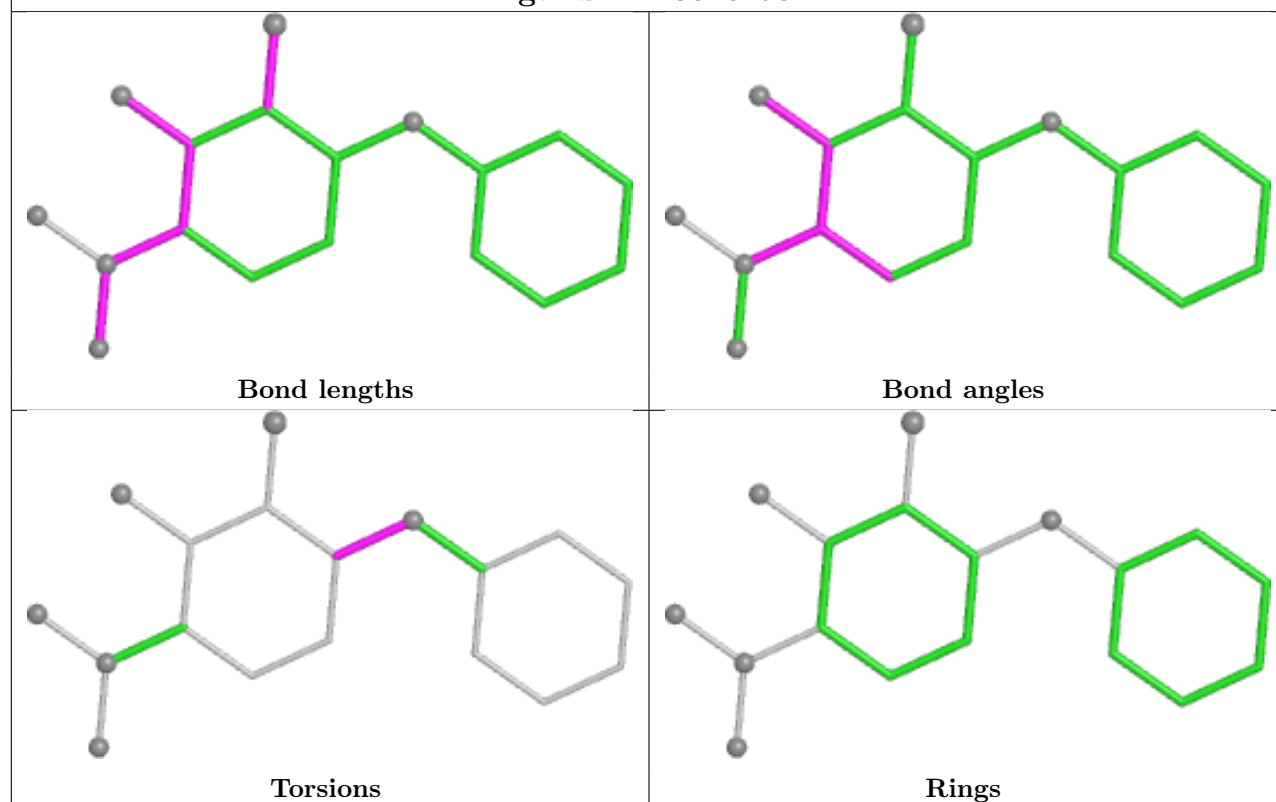
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	A1L38	1	0
2	C	501	A1L38	1	0

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 A1L38 D 501



Ligand A1L38 C 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	316/324 (97%)	0.53	14 (4%) 39 31	46, 67, 100, 115	0
1	B	302/324 (93%)	0.45	8 (2%) 57 51	50, 74, 102, 115	0
1	C	259/324 (79%)	0.52	7 (2%) 56 49	51, 72, 94, 113	0
1	D	240/324 (74%)	0.55	7 (2%) 53 46	52, 77, 117, 124	0
All	All	1117/1296 (86%)	0.51	36 (3%) 50 42	46, 72, 105, 124	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	CYS	3.6
1	C	293	ILE	3.4
1	B	105	SER	3.3
1	A	375	THR	3.3
1	C	211	LEU	3.1
1	A	326	THR	2.8
1	B	373	LEU	2.8
1	C	171	LEU	2.8
1	D	363	ILE	2.7
1	A	147	GLY	2.6
1	A	254	GLY	2.5
1	A	195	VAL	2.4
1	B	376	ALA	2.4
1	B	340	LEU	2.4
1	D	427	ILE	2.4
1	D	199	SER	2.3
1	A	269	LEU	2.3
1	A	209	HIS	2.3
1	B	324	ASP	2.3
1	C	197	ASP	2.3
1	A	169	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	212	TYR	2.3
1	C	325	PHE	2.3
1	A	134	VAL	2.2
1	D	201	MET	2.2
1	A	252	ALA	2.2
1	D	348	PRO	2.2
1	D	385	GLY	2.2
1	A	224	MET	2.2
1	C	316	PHE	2.2
1	D	352	ALA	2.1
1	C	375	THR	2.1
1	B	157	LEU	2.1
1	A	208	ILE	2.1
1	A	145	ALA	2.0
1	B	113	VAL	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](#)

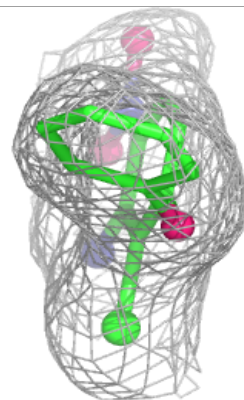
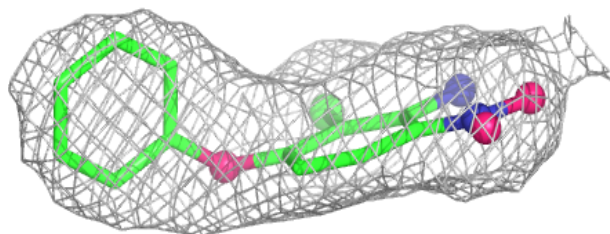
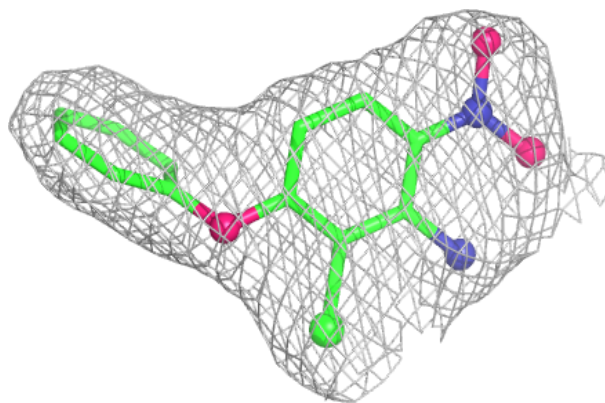
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1L38	C	501	18/18	0.95	0.08	46,54,61,61	0
2	A1L38	D	501	18/18	0.96	0.08	53,57,62,64	0

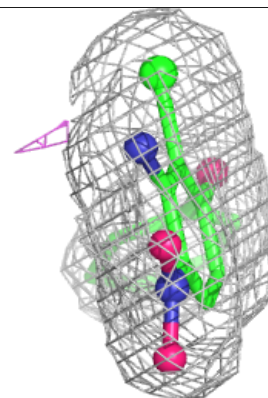
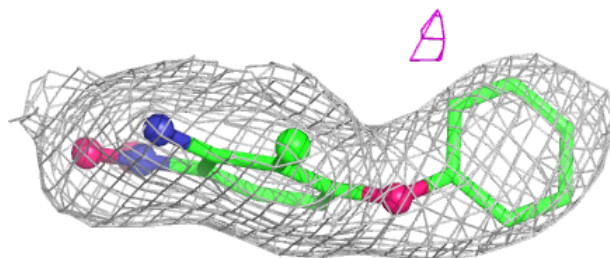
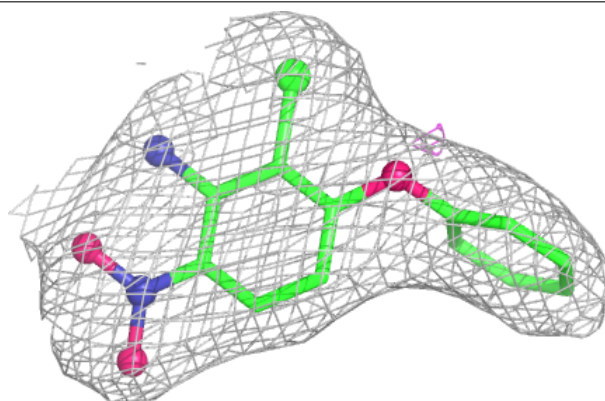
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1L38 C 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 A1L38 D 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.