



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:36 AM UTC

PDB ID : 5WDK / pdb_00005wdk
Title : A processive dipeptidyl aminopeptidase secreted from an established commensal bacterium *P. distasonis*
Authors : Wolan, D.W.; Xu, J.H.; Solania, A.; Chatterjee, S.; Jiang, Z.; ODonoghue, A.J.
Deposited on : 2017-07-05
Resolution : 2.36 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

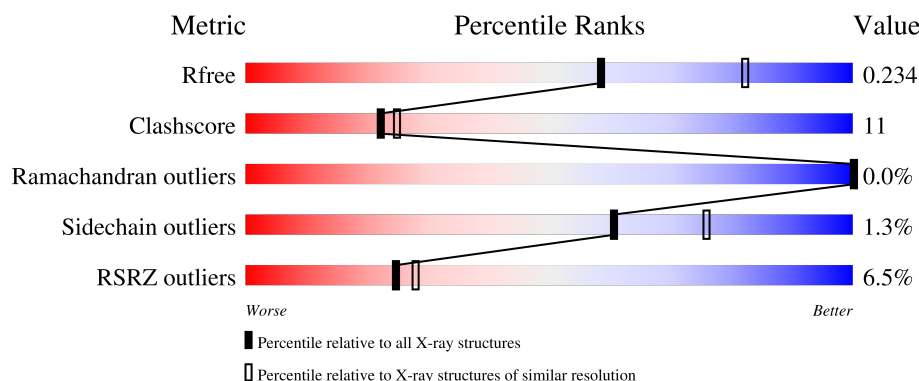
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	401	5% 78% 12% 9%
1	B	401	3% 70% 16% 14%
1	C	401	13% 65% 22% 12%
1	D	401	9% 66% 21% 9%

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Mol	Chain	Length	Quality of chain
1	E	401	
1	F	401	

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
3	T1O	B	502	-	X	-	-
3	T1O	E	503	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17403 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 Aminopeptidase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	1	0
			2821	1794	460	550	17			
1	B	345	Total	C	N	O	S	0	0	0
			2721	1733	442	529	17			
1	C	352	Total	C	N	O	S	0	0	0
			2715	1726	443	529	17			
1	D	363	Total	C	N	O	S	0	0	0
			2775	1764	449	545	17			
1	E	349	Total	C	N	O	S	0	0	0
			2739	1747	444	531	17			
1	F	374	Total	C	N	O	S	0	1	0
			2943	1873	481	572	17			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	expression tag	UNP A6LE66
A	6	GLY	-	expression tag	UNP A6LE66
A	7	SER	-	expression tag	UNP A6LE66
A	8	ASP	-	expression tag	UNP A6LE66
A	9	LYS	-	expression tag	UNP A6LE66
A	10	ILE	-	expression tag	UNP A6LE66
A	11	HIS	-	expression tag	UNP A6LE66
A	12	HIS	-	expression tag	UNP A6LE66
A	13	HIS	-	expression tag	UNP A6LE66
A	14	HIS	-	expression tag	UNP A6LE66
A	15	HIS	-	expression tag	UNP A6LE66
A	16	HIS	-	expression tag	UNP A6LE66
A	17	GLU	-	expression tag	UNP A6LE66
A	18	ASN	-	expression tag	UNP A6LE66
A	19	LEU	-	expression tag	UNP A6LE66
A	20	TYR	-	expression tag	UNP A6LE66
A	21	PHE	-	expression tag	UNP A6LE66

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLN	-	expression tag	UNP A6LE66
B	5	MET	-	expression tag	UNP A6LE66
B	6	GLY	-	expression tag	UNP A6LE66
B	7	SER	-	expression tag	UNP A6LE66
B	8	ASP	-	expression tag	UNP A6LE66
B	9	LYS	-	expression tag	UNP A6LE66
B	10	ILE	-	expression tag	UNP A6LE66
B	11	HIS	-	expression tag	UNP A6LE66
B	12	HIS	-	expression tag	UNP A6LE66
B	13	HIS	-	expression tag	UNP A6LE66
B	14	HIS	-	expression tag	UNP A6LE66
B	15	HIS	-	expression tag	UNP A6LE66
B	16	HIS	-	expression tag	UNP A6LE66
B	17	GLU	-	expression tag	UNP A6LE66
B	18	ASN	-	expression tag	UNP A6LE66
B	19	LEU	-	expression tag	UNP A6LE66
B	20	TYR	-	expression tag	UNP A6LE66
B	21	PHE	-	expression tag	UNP A6LE66
B	22	GLN	-	expression tag	UNP A6LE66
C	5	MET	-	expression tag	UNP A6LE66
C	6	GLY	-	expression tag	UNP A6LE66
C	7	SER	-	expression tag	UNP A6LE66
C	8	ASP	-	expression tag	UNP A6LE66
C	9	LYS	-	expression tag	UNP A6LE66
C	10	ILE	-	expression tag	UNP A6LE66
C	11	HIS	-	expression tag	UNP A6LE66
C	12	HIS	-	expression tag	UNP A6LE66
C	13	HIS	-	expression tag	UNP A6LE66
C	14	HIS	-	expression tag	UNP A6LE66
C	15	HIS	-	expression tag	UNP A6LE66
C	16	HIS	-	expression tag	UNP A6LE66
C	17	GLU	-	expression tag	UNP A6LE66
C	18	ASN	-	expression tag	UNP A6LE66
C	19	LEU	-	expression tag	UNP A6LE66
C	20	TYR	-	expression tag	UNP A6LE66
C	21	PHE	-	expression tag	UNP A6LE66
C	22	GLN	-	expression tag	UNP A6LE66
D	5	MET	-	expression tag	UNP A6LE66
D	6	GLY	-	expression tag	UNP A6LE66
D	7	SER	-	expression tag	UNP A6LE66
D	8	ASP	-	expression tag	UNP A6LE66
D	9	LYS	-	expression tag	UNP A6LE66

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Chain	Residue	Modelled	Actual	Comment	Reference
D	10	ILE	-	expression tag	UNP A6LE66
D	11	HIS	-	expression tag	UNP A6LE66
D	12	HIS	-	expression tag	UNP A6LE66
D	13	HIS	-	expression tag	UNP A6LE66
D	14	HIS	-	expression tag	UNP A6LE66
D	15	HIS	-	expression tag	UNP A6LE66
D	16	HIS	-	expression tag	UNP A6LE66
D	17	GLU	-	expression tag	UNP A6LE66
D	18	ASN	-	expression tag	UNP A6LE66
D	19	LEU	-	expression tag	UNP A6LE66
D	20	TYR	-	expression tag	UNP A6LE66
D	21	PHE	-	expression tag	UNP A6LE66
D	22	GLN	-	expression tag	UNP A6LE66
E	5	MET	-	expression tag	UNP A6LE66
E	6	GLY	-	expression tag	UNP A6LE66
E	7	SER	-	expression tag	UNP A6LE66
E	8	ASP	-	expression tag	UNP A6LE66
E	9	LYS	-	expression tag	UNP A6LE66
E	10	ILE	-	expression tag	UNP A6LE66
E	11	HIS	-	expression tag	UNP A6LE66
E	12	HIS	-	expression tag	UNP A6LE66
E	13	HIS	-	expression tag	UNP A6LE66
E	14	HIS	-	expression tag	UNP A6LE66
E	15	HIS	-	expression tag	UNP A6LE66
E	16	HIS	-	expression tag	UNP A6LE66
E	17	GLU	-	expression tag	UNP A6LE66
E	18	ASN	-	expression tag	UNP A6LE66
E	19	LEU	-	expression tag	UNP A6LE66
E	20	TYR	-	expression tag	UNP A6LE66
E	21	PHE	-	expression tag	UNP A6LE66
E	22	GLN	-	expression tag	UNP A6LE66
F	5	MET	-	expression tag	UNP A6LE66
F	6	GLY	-	expression tag	UNP A6LE66
F	7	SER	-	expression tag	UNP A6LE66
F	8	ASP	-	expression tag	UNP A6LE66
F	9	LYS	-	expression tag	UNP A6LE66
F	10	ILE	-	expression tag	UNP A6LE66
F	11	HIS	-	expression tag	UNP A6LE66
F	12	HIS	-	expression tag	UNP A6LE66
F	13	HIS	-	expression tag	UNP A6LE66
F	14	HIS	-	expression tag	UNP A6LE66
F	15	HIS	-	expression tag	UNP A6LE66

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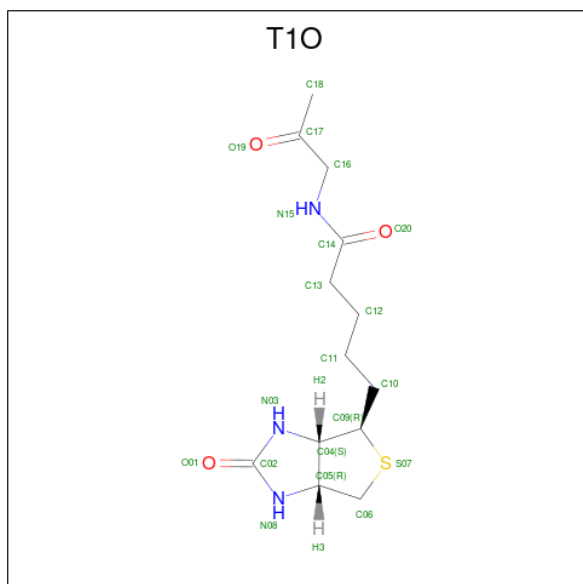
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Chain	Residue	Modelled	Actual	Comment	Reference
F	16	HIS	-	expression tag	UNP A6LE66
F	17	GLU	-	expression tag	UNP A6LE66
F	18	ASN	-	expression tag	UNP A6LE66
F	19	LEU	-	expression tag	UNP A6LE66
F	20	TYR	-	expression tag	UNP A6LE66
F	21	PHE	-	expression tag	UNP A6LE66
F	22	GLN	-	expression tag	UNP A6LE66

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	B	1	Total K 1 1	0	0
2	C	2	Total K 2 2	0	0
2	D	2	Total K 2 2	0	0
2	E	2	Total K 2 2	0	0
2	F	2	Total K 2 2	0	0

- Molecule 3 is 5-[(3aS,4R,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]-N-(2-oxopropyl)pentanamide (CCD ID: T1O) (formula: C₁₃H₂₁N₃O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 20	C 13	N 3	O 3	S 1	0	0
3	B	1	Total 20	C 13	N 3	O 3	S 1	0	0
3	C	1	Total 20	C 13	N 3	O 3	S 1	0	0
3	D	1	Total 20	C 13	N 3	O 3	S 1	0	0
3	E	1	Total 20	C 13	N 3	O 3	S 1	0	0
3	F	1	Total 20	C 13	N 3	O 3	S 1	0	0

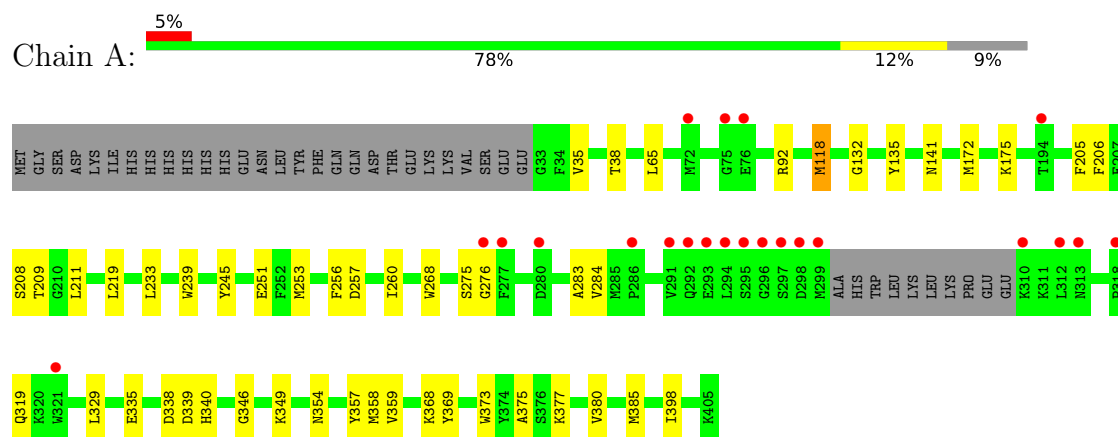
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total 97	O 97	0	0
4	B	97	Total 97	O 97	0	0
4	C	45	Total 45	O 45	0	0
4	D	49	Total 49	O 49	0	0
4	E	137	Total 137	O 137	0	0
4	F	133	Total 133	O 133	0	0

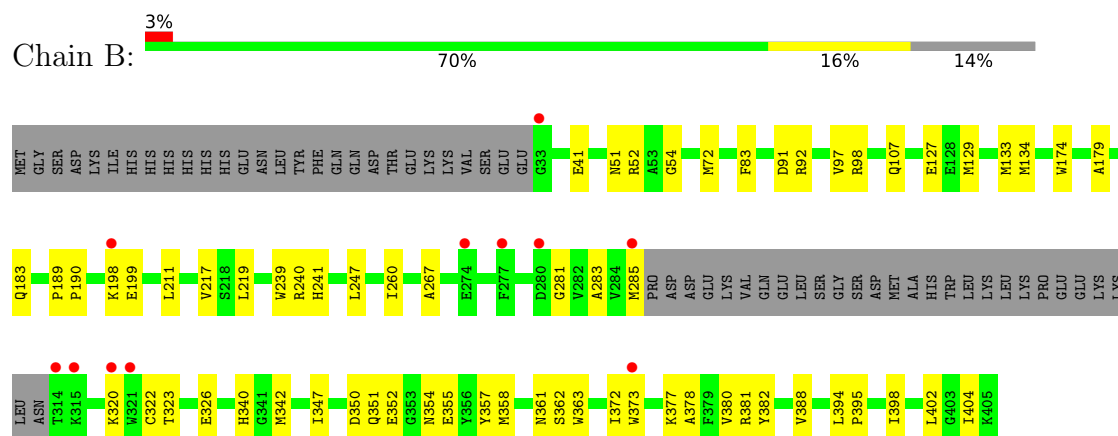
3 Residue-property plots [i](#)

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.

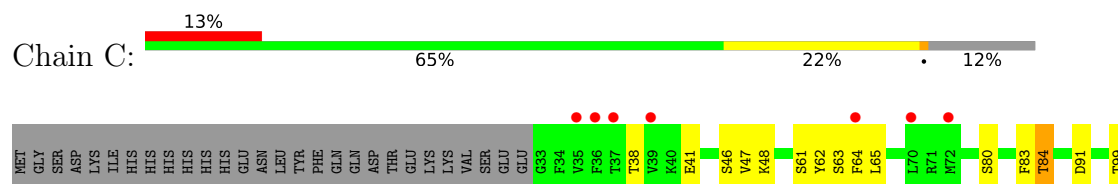
• Molecule 1: Aminopeptidase C

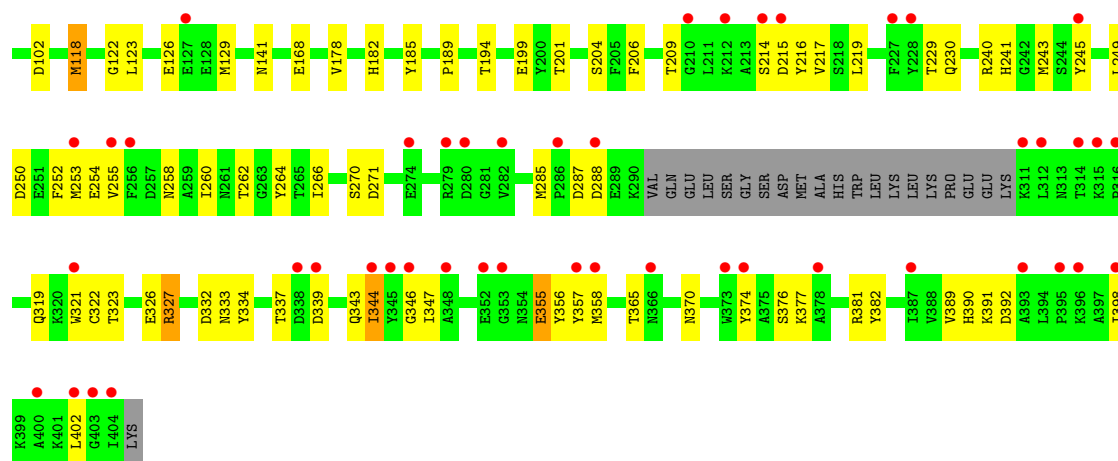


• Molecule 1: Aminopeptidase C

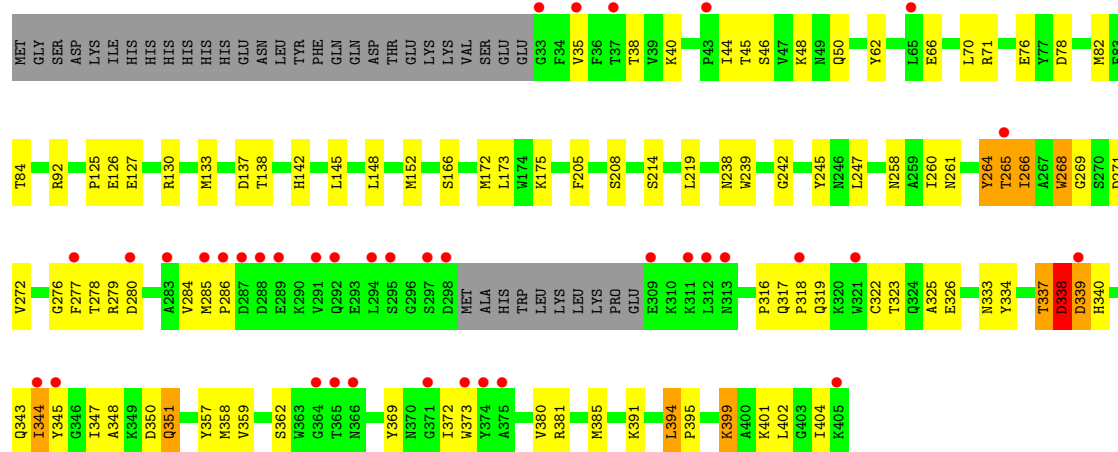


• Molecule 1: Aminopeptidase C

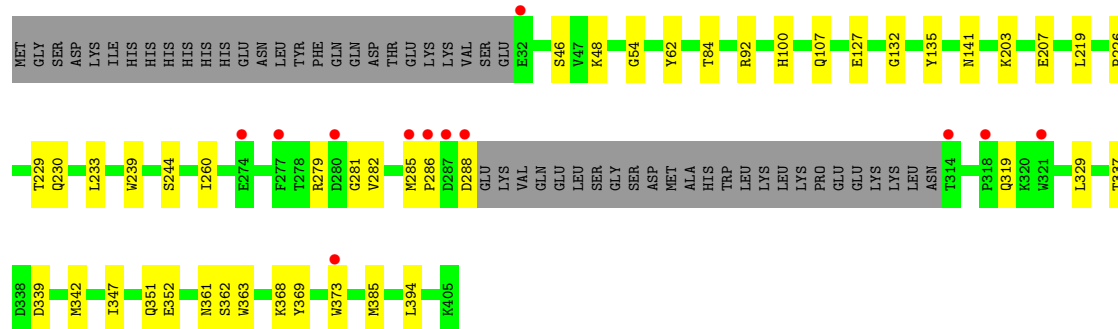
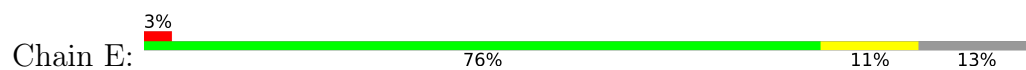




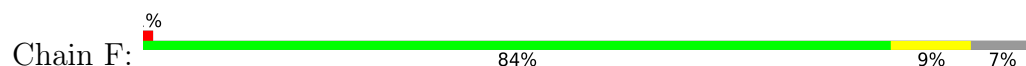
• Molecule 1: Aminopeptidase C

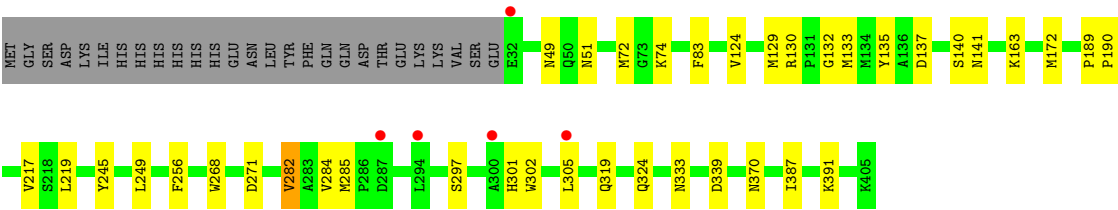


• Molecule 1: Aminopeptidase C



• Molecule 1: Aminopeptidase C





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.91Å 136.97Å 208.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.10 – 2.36 50.10 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.10-2.36) 98.9 (50.10-2.36)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.186 , 0.231 0.191 , 0.234	Depositor DCC
R_{free} test set	6069 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17403	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: T1O, K

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	0.47	0/2897	0.54	0/3935
1	B	0.47	1/2793 (0.0%)	0.55	1/3790 (0.0%)
1	C	0.43	0/2786	0.62	1/3792 (0.0%)
1	D	0.50	0/2846	0.66	6/3873 (0.2%)
1	E	0.45	0/2812	0.58	3/3817 (0.1%)
1	F	0.49	1/3024 (0.0%)	0.60	2/4104 (0.0%)
All	All	0.47	2/17158 (0.0%)	0.59	13/23311 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	268	TRP	C-N	-5.32	1.31	1.33
1	B	51	ASN	C-O	-5.04	1.19	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	338	ASP	N-CA-C	8.68	121.69	111.71
1	D	337	THR	N-CA-C	7.79	123.54	113.18
1	B	52	ARG	N-CA-C	7.58	120.99	109.62
1	E	282	VAL	N-CA-C	7.04	118.19	107.77
1	F	333	ASN	N-CA-C	7.01	121.55	112.92
1	C	327	ARG	N-CA-C	6.81	118.49	111.14
1	D	264	TYR	N-CA-C	6.10	119.50	110.48
1	E	279	ARG	N-CA-C	6.08	117.57	111.07
1	D	266	ILE	N-CA-C	6.05	116.65	108.17
1	E	282	VAL	CB-CA-C	-5.62	102.83	110.42
1	F	140	SER	N-CA-C	5.59	118.55	110.28
1	D	268	TRP	N-CA-C	5.28	117.58	109.07
1	D	339	ASP	N-CA-C	5.00	118.30	111.39

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	2821	0	2601	32	0
1	B	2721	0	2543	44	0
1	C	2715	0	2480	86	0
1	D	2775	0	2518	127	0
1	E	2739	0	2556	35	0
1	F	2943	0	2751	25	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	0	0
3	F	20	0	0	0	0
4	A	97	0	0	1	0
4	B	97	0	0	1	0
4	C	45	0	0	0	0
4	D	49	0	0	1	0
4	E	137	0	0	2	0
4	F	133	0	0	1	0
All	All	17403	0	15449	343	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (343) 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:394:LEU:HB3	1:D:399:LYS:CE	1.29	1.61
1:D:394:LEU:HB3	1:D:399:LYS:NZ	1.11	1.40
1:D:394:LEU:CB	1:D:399:LYS:CE	2.04	1.35
1:D:345:TYR:CE2	1:D:372:ILE:HD11	1.62	1.33
1:D:266:ILE:HB	1:D:344:ILE:CG2	1.58	1.32
1:D:394:LEU:CB	1:D:399:LYS:NZ	1.94	1.30
1:D:265:THR:CG2	1:D:343:GLN:HE21	1.51	1.21
1:D:394:LEU:CB	1:D:399:LYS:HZ1	1.51	1.19
1:D:265:THR:HG21	1:D:343:GLN:NE2	1.62	1.12
1:D:265:THR:HG21	1:D:343:GLN:HE21	1.02	1.09
1:D:347:ILE:O	1:D:358:MET:HE2	1.54	1.08
1:D:394:LEU:HB3	1:D:399:LYS:HE2	1.36	1.01
1:D:345:TYR:HE2	1:D:372:ILE:HD11	0.87	1.00
1:C:41:GLU:HG2	1:C:358:MET:HE1	1.44	0.99
1:C:64:PHE:HA	1:C:343:GLN:NE2	1.80	0.97
1:D:344:ILE:HD12	1:D:357:TYR:HB3	1.48	0.95
1:D:345:TYR:HE2	1:D:372:ILE:CD1	1.79	0.95
1:D:266:ILE:HB	1:D:344:ILE:HG23	1.49	0.93
1:E:281:GLY:O	1:E:373:TRP:HB2	1.71	0.91
1:D:266:ILE:HB	1:D:344:ILE:HG21	1.50	0.89
1:D:394:LEU:CG	1:D:399:LYS:NZ	2.34	0.89
1:D:238:ASN:HD21	1:D:242:GLY:H	1.16	0.89
1:D:344:ILE:CD1	1:D:357:TYR:HB3	2.03	0.88
1:C:260:ILE:HD11	1:C:344:ILE:CD1	2.03	0.88
1:C:64:PHE:N	1:C:343:GLN:HE21	1.71	0.88
1:D:394:LEU:CB	1:D:399:LYS:HE2	1.92	0.88
1:C:63:SER:C	1:C:343:GLN:NE2	2.33	0.87
1:D:278:THR:HG22	1:D:280:ASP:H	1.41	0.86
1:D:394:LEU:HB2	1:D:399:LYS:CE	2.05	0.86
1:D:394:LEU:CB	1:D:399:LYS:HE3	2.03	0.86
1:B:285:MET:HE1	1:B:382:TYR:HB2	1.60	0.84
1:A:346:GLY:HA3	1:A:358:MET:HE3	1.62	0.81
1:C:64:PHE:CA	1:C:343:GLN:NE2	2.43	0.81
1:D:265:THR:HG23	1:D:343:GLN:HE21	1.45	0.81
1:D:345:TYR:CE2	1:D:372:ILE:CD1	2.57	0.80
1:D:278:THR:HG21	1:D:280:ASP:OD2	1.81	0.80
1:D:344:ILE:HD11	1:D:357:TYR:CD1	2.16	0.79
1:C:260:ILE:HD11	1:C:344:ILE:HD13	1.63	0.79
1:D:347:ILE:HG22	1:D:348:ALA:N	1.99	0.78
1:F:285:MET:H	1:F:319:GLN:HE22	1.32	0.77
1:D:271:ASP:OD1	1:D:338:ASP:OD2	2.03	0.77
1:D:265:THR:CG2	1:D:343:GLN:NE2	2.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:LEU:HB3	1:D:399:LYS:HZ1	0.93	0.76
1:C:64:PHE:CA	1:C:343:GLN:HE21	1.98	0.76
1:D:394:LEU:HB2	1:D:399:LYS:HE3	1.67	0.75
1:D:284:VAL:HG22	1:D:319:GLN:HE22	1.51	0.74
1:E:342:MET:HE1	1:E:373:TRP:HE1	1.51	0.74
1:D:345:TYR:CZ	1:D:372:ILE:HD11	2.22	0.73
1:E:342:MET:HE3	1:E:361:ASN:CG	2.13	0.73
1:C:64:PHE:N	1:C:343:GLN:NE2	2.36	0.73
1:D:394:LEU:CG	1:D:399:LYS:HZ2	2.03	0.72
1:D:35:VAL:N	1:D:351:GLN:OE1	2.21	0.72
1:D:266:ILE:HB	1:D:344:ILE:HG22	1.68	0.72
1:D:394:LEU:CG	1:D:399:LYS:HZ1	2.01	0.71
1:D:347:ILE:O	1:D:358:MET:CE	2.35	0.71
1:B:340:HIS:HE2	1:B:363:TRP:HZ2	1.36	0.71
1:C:46:SER:O	1:C:48:LYS:NZ	2.24	0.70
1:E:54:GLY:H	1:E:107:GLN:NE2	1.89	0.70
1:C:358:MET:HG2	1:C:374:TYR:HE1	1.55	0.69
1:B:395:PRO:HG2	1:B:398:ILE:HD12	1.75	0.69
1:D:71:ARG:CZ	1:D:264:TYR:HE1	2.05	0.69
1:C:258:ASN:O	1:C:262:THR:HG22	1.92	0.69
1:C:214:SER:O	1:C:391:LYS:HE2	1.92	0.69
1:B:361:ASN:ND2	1:B:362:SER:H	1.92	0.68
1:D:266:ILE:CB	1:D:344:ILE:CG2	2.55	0.68
1:D:38:THR:HG23	1:D:358:MET:HE1	1.74	0.68
1:C:358:MET:HG2	1:C:374:TYR:CE1	2.30	0.67
1:C:201:THR:CG2	1:C:204:SER:H	2.08	0.67
1:B:361:ASN:HD22	1:B:362:SER:H	1.42	0.67
1:B:41:GLU:HB3	1:B:358:MET:CE	2.25	0.67
1:E:342:MET:HE1	1:E:373:TRP:NE1	2.10	0.67
1:C:260:ILE:HG21	1:C:347:ILE:HG13	1.75	0.66
1:A:206:PHE:O	1:A:209:THR:OG1	2.11	0.66
1:A:257:ASP:OD1	1:A:357:TYR:OH	2.07	0.65
1:E:285:MET:H	1:E:319:GLN:HE22	1.44	0.65
1:F:130:ARG:H	1:F:133:MET:HE3	1.61	0.65
1:B:129:MET:HE2	1:B:190:PRO:HD3	1.78	0.64
1:B:83:PHE:HB2	1:B:129:MET:HE3	1.79	0.64
1:F:297:SER:HB2	1:F:301:HIS:HB2	1.79	0.64
1:C:230:GLN:HB3	1:C:243:MET:HG2	1.79	0.64
1:E:337:THR:C	1:E:385:MET:HE1	2.23	0.63
1:D:347:ILE:CG2	1:D:348:ALA:N	2.62	0.63
1:C:262:THR:HG23	1:C:264:TYR:CD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:LEU:HD23	1:D:245:TYR:HB2	1.81	0.63
1:C:91:ASP:OD2	1:C:240:ARG:NH2	2.31	0.62
1:F:249:LEU:H	1:F:324:GLN:HE22	1.47	0.62
1:D:40:LYS:NZ	1:D:261:ASN:O	2.33	0.62
1:C:62:TYR:OH	1:C:84:THR:HG21	1.99	0.62
1:C:118:MET:HB2	1:C:123:LEU:HD21	1.80	0.62
1:C:201:THR:HG23	1:C:204:SER:H	1.63	0.62
1:C:321:TRP:CH2	1:C:377:LYS:HB2	2.34	0.62
1:B:247:LEU:HD21	1:B:402:LEU:HD11	1.80	0.62
1:C:390:HIS:HD2	1:C:392:ASP:H	1.45	0.62
1:C:253:MET:HE2	1:C:253:MET:HA	1.81	0.61
1:D:323:THR:HG22	1:D:326:GLU:HG3	1.81	0.61
1:D:316:PRO:HG2	1:D:351:GLN:HE22	1.65	0.61
1:A:118:MET:HG3	1:A:206:PHE:CE1	2.36	0.60
1:D:344:ILE:HG23	1:D:344:ILE:O	1.99	0.60
1:C:266:ILE:HB	1:C:344:ILE:CG2	2.31	0.60
1:D:322:CYS:O	1:D:381:ARG:NH2	2.31	0.60
1:E:203:LYS:O	1:E:207:GLU:HG3	2.00	0.60
1:C:357:TYR:CE2	1:C:377:LYS:HD3	2.37	0.60
1:D:394:LEU:HG	1:D:399:LYS:NZ	2.15	0.59
1:F:285:MET:H	1:F:319:GLN:NE2	1.98	0.59
1:A:209:THR:HB	1:A:211:LEU:HG	1.85	0.59
1:C:249:LEU:HD11	1:C:381:ARG:HG3	1.85	0.59
1:D:344:ILE:HD11	1:D:357:TYR:CG	2.37	0.59
1:B:281:GLY:O	1:B:373:TRP:HB2	2.03	0.58
1:C:250:ASP:O	1:C:254:GLU:HG3	2.03	0.58
1:D:316:PRO:O	1:D:317:GLN:HG3	2.03	0.58
1:D:268:TRP:CZ2	1:D:380:VAL:HG22	2.37	0.58
1:F:83:PHE:HD1	1:F:129:MET:HE1	1.68	0.58
1:C:129:MET:HE1	1:C:189:PRO:HA	1.86	0.58
1:C:322:CYS:O	1:C:381:ARG:NH2	2.34	0.58
1:C:83:PHE:HD2	1:C:84:THR:HG22	1.68	0.57
1:D:284:VAL:HG13	1:D:286:PRO:HD3	1.86	0.57
1:D:214:SER:O	1:D:391:LYS:HE3	2.04	0.57
1:D:345:TYR:OH	1:D:372:ILE:CD1	2.53	0.57
1:C:262:THR:HG23	1:C:264:TYR:HD1	1.68	0.57
1:B:54:GLY:H	1:B:107:GLN:NE2	2.02	0.57
1:C:219:LEU:HD13	1:C:245:TYR:HB2	1.87	0.57
1:D:92:ARG:HG3	1:D:239:TRP:CE2	2.40	0.56
1:E:62:TYR:HH	1:E:84:THR:HG1	1.52	0.56
1:D:44:ILE:HD12	1:D:45:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:TYR:OH	1:D:372:ILE:HG12	2.05	0.56
1:B:323:THR:OG1	1:B:326:GLU:HG3	2.06	0.56
1:D:316:PRO:HG2	1:D:351:GLN:NE2	2.21	0.56
1:D:166:SER:HB3	1:D:172:MET:HE1	1.88	0.56
1:D:238:ASN:ND2	1:D:242:GLY:H	1.97	0.56
1:D:247:LEU:HD21	1:D:402:LEU:HD21	1.87	0.56
1:B:41:GLU:HB3	1:B:358:MET:HE1	1.88	0.56
1:D:148:LEU:O	1:D:152:MET:HG3	2.06	0.55
1:A:283:ALA:HB3	1:A:375:ALA:HA	1.88	0.55
1:A:92:ARG:HB2	1:A:239:TRP:CZ2	2.41	0.55
1:A:205:PHE:O	1:A:208:SER:HB3	2.07	0.55
1:C:206:PHE:O	1:C:209:THR:HG22	2.06	0.55
1:D:344:ILE:CD1	1:D:357:TYR:CB	2.82	0.55
1:D:394:LEU:C	1:D:399:LYS:HE2	2.32	0.55
1:E:219:LEU:HD11	1:E:394:LEU:HD21	1.88	0.55
1:B:217:VAL:HG11	1:B:404:ILE:HD13	1.87	0.55
1:D:46:SER:O	1:D:48:LYS:HE2	2.07	0.54
1:A:256:PHE:O	1:A:260:ILE:HG22	2.06	0.54
1:A:260:ILE:HD11	1:A:346:GLY:CA	2.37	0.54
1:B:267:ALA:HB3	1:B:388:VAL:HB	1.90	0.54
1:C:178:VAL:O	1:C:182:HIS:HD2	1.90	0.54
1:D:78:ASP:OD2	1:D:126:GLU:HG3	2.07	0.54
1:D:369:TYR:HB2	1:D:372:ILE:HG22	1.89	0.54
1:D:394:LEU:HD23	1:D:399:LYS:HZ2	1.72	0.54
1:D:82:MET:HE1	1:D:142:HIS:CE1	2.43	0.54
1:D:166:SER:HB3	1:D:172:MET:CE	2.38	0.54
1:E:342:MET:CE	1:E:373:TRP:HE1	2.21	0.53
1:C:260:ILE:HD12	1:C:346:GLY:HA2	1.91	0.53
1:B:133:MET:HG3	1:B:134:MET:HE3	1.90	0.53
1:C:285:MET:H	1:C:319:GLN:HE22	1.55	0.53
1:D:337:THR:C	1:D:385:MET:HE1	2.34	0.53
1:A:284:VAL:HB	1:A:319:GLN:HE22	1.73	0.53
1:B:134:MET:HE2	1:B:134:MET:HA	1.89	0.53
1:C:287:ASP:OD1	1:C:288:ASP:N	2.41	0.53
1:C:327:ARG:HA	1:C:382:TYR:HE1	1.74	0.53
1:D:339:ASP:H	1:D:385:MET:HE1	1.74	0.52
1:D:394:LEU:CD2	1:D:399:LYS:HZ2	2.21	0.52
1:E:285:MET:HE3	1:E:286:PRO:HD2	1.91	0.52
1:C:47:VAL:HB	1:C:365:THR:HG22	1.90	0.52
1:F:129:MET:HE2	1:F:190:PRO:HD3	1.89	0.52
1:A:65:LEU:HD22	1:A:118:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:SER:O	1:C:343:GLN:NE2	2.31	0.52
1:C:365:THR:O	1:C:370:ASN:HA	2.09	0.52
1:D:137:ASP:OD1	1:D:138:THR:N	2.43	0.52
1:F:249:LEU:H	1:F:324:GLN:NE2	2.08	0.52
1:C:229:THR:HG22	1:C:230:GLN:H	1.75	0.52
1:B:285:MET:HE3	1:B:320:LYS:O	2.10	0.51
1:D:50:GLN:HG2	1:D:362:SER:O	2.10	0.51
1:C:355:GLU:HB3	1:C:377:LYS:HE2	1.92	0.51
1:D:339:ASP:H	1:D:385:MET:CE	2.24	0.51
1:D:71:ARG:NE	1:D:264:TYR:CE1	2.79	0.51
1:D:344:ILE:CD1	1:D:357:TYR:CG	2.94	0.51
1:E:226:PRO:O	1:E:229:THR:OG1	2.28	0.51
1:A:172:MET:HB2	1:A:175:LYS:HG3	1.93	0.51
1:C:217:VAL:HG23	1:C:219:LEU:HD21	1.93	0.51
1:D:172:MET:HB2	1:D:175:LYS:HG3	1.91	0.51
1:D:219:LEU:HD11	1:D:394:LEU:HD11	1.91	0.51
1:B:98:ARG:NH1	1:C:332:ASP:OD1	2.34	0.51
1:C:215:ASP:O	1:C:391:LYS:HG3	2.11	0.51
1:D:266:ILE:CB	1:D:344:ILE:HG21	2.34	0.51
1:B:357:TYR:CE2	1:B:377:LYS:HD2	2.47	0.50
1:C:219:LEU:CD1	1:C:245:TYR:HB2	2.41	0.50
1:C:65:LEU:HD13	1:C:118:MET:HE1	1.93	0.50
1:F:370:ASN:ND2	4:F:607:HOH:O	2.45	0.50
1:D:62:TYR:OH	1:D:84:THR:OG1	2.17	0.50
1:D:142:HIS:HB3	1:D:145:LEU:HD23	1.94	0.50
1:D:238:ASN:ND2	4:D:601:HOH:O	2.35	0.50
1:D:271:ASP:HA	1:D:338:ASP:OD2	2.12	0.50
1:A:359:VAL:CG1	1:A:373:TRP:HB2	2.42	0.50
1:B:127:GLU:CD	1:B:127:GLU:H	2.20	0.50
1:D:344:ILE:HD11	1:D:357:TYR:HB3	1.90	0.50
1:D:351:GLN:CD	1:D:351:GLN:H	2.19	0.50
1:C:252:PHE:O	1:C:255:VAL:HG12	2.10	0.50
1:A:253:MET:HE1	1:A:380:VAL:HG12	1.93	0.49
1:D:260:ILE:HG21	1:D:347:ILE:HG13	1.93	0.49
1:E:48:LYS:HD2	4:E:733:HOH:O	2.12	0.49
1:B:91:ASP:OD2	1:B:240:ARG:NH2	2.45	0.49
1:D:127:GLU:CD	1:D:127:GLU:H	2.21	0.49
1:C:323:THR:OG1	1:C:326:GLU:HG3	2.12	0.49
1:C:83:PHE:CD2	1:C:84:THR:HG22	2.47	0.49
1:F:141:ASN:C	1:F:141:ASN:HD22	2.21	0.49
1:D:278:THR:HG22	1:D:279:ARG:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:PHE:HB2	1:F:129:MET:HE3	1.96	0.48
1:D:323:THR:CG2	1:D:326:GLU:H	2.26	0.48
1:E:54:GLY:H	1:E:107:GLN:HE21	1.59	0.48
1:A:38:THR:HG23	1:A:358:MET:HE1	1.95	0.48
1:C:356:TYR:C	1:C:377:LYS:NZ	2.71	0.48
1:F:282:VAL:HG13	1:F:284:VAL:HG13	1.95	0.48
1:A:219:LEU:HD23	1:A:245:TYR:HB2	1.96	0.47
1:C:122:GLY:O	1:C:123:LEU:HD23	2.13	0.47
1:B:198:LYS:HD2	1:B:199:GLU:H	1.79	0.47
1:A:132:GLY:HA2	1:A:135:TYR:CZ	2.48	0.47
1:B:355:GLU:HB3	1:B:377:LYS:HG2	1.96	0.47
1:C:141:ASN:C	1:C:141:ASN:HD22	2.21	0.47
1:C:253:MET:HG3	1:C:381:ARG:HB2	1.97	0.47
1:E:351:GLN:HG2	1:E:352:GLU:HG2	1.96	0.47
1:A:175:LYS:NZ	4:A:604:HOH:O	2.47	0.47
1:A:251:GLU:HB3	1:A:398:ILE:HD11	1.95	0.47
1:C:266:ILE:HG23	1:C:389:VAL:HG13	1.96	0.47
1:C:356:TYR:O	1:C:377:LYS:NZ	2.46	0.47
1:D:130:ARG:H	1:D:133:MET:HE3	1.78	0.47
1:D:284:VAL:HG22	1:D:319:GLN:NE2	2.26	0.47
1:D:125:PRO:HG3	1:D:205:PHE:CZ	2.49	0.47
1:D:323:THR:HG23	1:D:325:ALA:H	1.80	0.47
1:E:132:GLY:HA2	1:E:135:TYR:CE1	2.50	0.47
1:B:219:LEU:HD11	1:B:394:LEU:HD21	1.97	0.47
1:E:368:LYS:HD3	1:E:369:TYR:CZ	2.50	0.47
1:F:49:ASN:ND2	1:F:51:ASN:H	2.12	0.47
1:B:355:GLU:HB3	1:B:377:LYS:CG	2.45	0.46
1:A:268:TRP:CZ2	1:A:380:VAL:HG22	2.51	0.46
1:B:283:ALA:HB2	1:B:373:TRP:HZ3	1.81	0.46
1:B:342:MET:HE2	1:B:361:ASN:CG	2.40	0.46
1:C:38:THR:HG21	1:C:41:GLU:HG3	1.97	0.46
1:C:63:SER:C	1:C:343:GLN:HE21	2.04	0.46
1:B:357:TYR:CZ	1:B:377:LYS:HE3	2.50	0.46
1:D:71:ARG:NE	1:D:264:TYR:HE1	2.14	0.46
1:D:394:LEU:HG	1:D:399:LYS:HZ2	1.77	0.46
1:A:276:GLY:HA3	1:A:284:VAL:O	2.15	0.46
1:D:172:MET:HE1	1:E:329:LEU:CD1	2.45	0.46
1:A:260:ILE:HD11	1:A:346:GLY:HA2	1.98	0.46
1:B:92:ARG:HG3	1:B:239:TRP:CE2	2.51	0.46
1:C:61:SER:O	1:C:65:LEU:HG	2.16	0.46
1:D:391:LYS:HD3	1:D:404:ILE:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:GLY:HA2	1:E:135:TYR:CZ	2.51	0.46
1:C:327:ARG:HA	1:C:382:TYR:CE1	2.51	0.46
1:D:78:ASP:CG	1:D:126:GLU:HG3	2.41	0.45
1:E:342:MET:HE1	1:E:373:TRP:CE2	2.51	0.45
1:D:323:THR:HG23	1:D:325:ALA:N	2.31	0.45
1:C:214:SER:O	1:C:391:LYS:CE	2.63	0.45
1:E:260:ILE:HG21	1:E:347:ILE:HG13	1.98	0.45
1:D:278:THR:CG2	1:D:280:ASP:H	2.23	0.45
1:C:83:PHE:HA	1:C:129:MET:SD	2.57	0.45
1:F:132:GLY:HA2	1:F:135:TYR:CE1	2.52	0.45
1:D:258:ASN:HD22	1:D:395:PRO:HG3	1.82	0.45
1:A:368:LYS:HG2	1:A:369:TYR:CE1	2.51	0.44
1:D:285:MET:O	1:D:319:GLN:HB2	2.16	0.44
1:D:345:TYR:CD1	1:D:345:TYR:O	2.70	0.44
1:C:168:GLU:OE1	1:C:168:GLU:N	2.49	0.44
1:D:333:ASN:O	1:D:334:TYR:HB2	2.18	0.44
1:F:256:PHE:CZ	1:F:387:ILE:HG21	2.53	0.44
1:B:72:MET:HE1	1:B:211:LEU:HD23	1.99	0.44
1:D:70:LEU:HD21	1:D:76:GLU:HA	1.99	0.44
1:F:271:ASP:HA	1:F:339:ASP:HB2	1.99	0.44
1:B:260:ILE:HG21	1:B:347:ILE:HG12	2.00	0.44
1:B:322:CYS:SG	1:B:381:ARG:HG2	2.57	0.44
1:D:71:ARG:NH2	1:D:264:TYR:HE1	2.16	0.44
1:D:238:ASN:HD21	1:D:242:GLY:N	1.98	0.44
1:E:92:ARG:HB2	1:E:239:TRP:CZ2	2.52	0.44
1:E:362:SER:C	1:E:363:TRP:HD1	2.26	0.44
1:C:333:ASN:O	1:C:334:TYR:HB2	2.16	0.44
1:C:230:GLN:HB3	1:C:243:MET:CG	2.46	0.43
1:E:233:LEU:HD23	1:E:233:LEU:HA	1.86	0.43
1:F:217:VAL:HG13	1:F:391:LYS:HG2	2.00	0.43
1:C:337:THR:OG1	1:C:339:ASP:OD1	2.36	0.43
1:A:335:GLU:OE2	1:F:163:LYS:HD2	2.19	0.43
1:C:194:THR:HA	1:C:199:GLU:HA	1.99	0.43
1:E:46:SER:OG	1:E:48:LYS:HE3	2.18	0.43
1:E:339:ASP:HA	1:E:385:MET:HE3	1.99	0.43
1:D:359:VAL:HG23	1:D:373:TRP:HB2	1.99	0.43
1:C:344:ILE:HD13	1:C:344:ILE:C	2.44	0.43
1:F:302:TRP:HA	1:F:305:LEU:HD22	2.00	0.43
1:E:230:GLN:HA	1:E:244:SER:O	2.18	0.43
1:A:349:LYS:HA	1:A:354:ASN:O	2.18	0.43
1:D:316:PRO:HB3	1:D:350:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:HIS:CE1	1:C:241:HIS:NE2	2.86	0.42
1:D:284:VAL:CG2	1:D:319:GLN:HE22	2.27	0.42
1:B:129:MET:CE	1:B:189:PRO:HA	2.49	0.42
1:D:62:TYR:O	1:D:66:GLU:HG3	2.18	0.42
1:D:316:PRO:CG	1:D:351:GLN:HE22	2.31	0.42
1:E:141:ASN:C	1:E:141:ASN:HD22	2.25	0.42
1:A:233:LEU:HD23	1:A:233:LEU:HA	1.90	0.42
1:A:338:ASP:O	1:A:340:HIS:N	2.52	0.42
1:C:216:TYR:CE1	1:C:390:HIS:HB2	2.54	0.42
1:C:402:LEU:HA	1:C:402:LEU:HD22	1.78	0.42
1:F:72:MET:HE3	1:F:74:LYS:NZ	2.34	0.42
1:A:377:LYS:HB2	1:A:377:LYS:HE2	1.74	0.42
1:C:185:TYR:CD2	1:D:173:LEU:HD23	2.55	0.42
1:C:260:ILE:HD12	1:C:346:GLY:CA	2.49	0.42
1:E:342:MET:HE1	1:E:373:TRP:CZ2	2.55	0.42
1:D:345:TYR:OH	1:D:372:ILE:CG1	2.67	0.42
1:B:179:ALA:O	1:B:183:GLN:HG3	2.19	0.42
1:D:269:GLY:HA2	1:D:340:HIS:O	2.20	0.42
1:F:129:MET:CE	1:F:189:PRO:HA	2.50	0.42
1:B:350:ASP:OD2	1:B:354:ASN:HB2	2.21	0.41
1:B:361:ASN:HD22	1:B:362:SER:N	2.13	0.41
1:B:361:ASN:HB3	4:B:640:HOH:O	2.20	0.41
1:C:356:TYR:HA	1:C:376:SER:HA	2.02	0.41
1:D:272:VAL:HB	1:D:277:PHE:CD2	2.55	0.41
1:B:357:TYR:HD2	1:B:380:VAL:HG21	1.85	0.41
1:C:229:THR:HG22	1:C:230:GLN:N	2.35	0.41
1:D:71:ARG:CZ	1:D:264:TYR:CE1	2.95	0.41
1:E:337:THR:O	1:E:385:MET:HE1	2.20	0.41
1:B:351:GLN:HG2	1:B:352:GLU:HG3	2.02	0.41
1:C:260:ILE:HG23	1:C:346:GLY:HA2	2.01	0.41
1:E:285:MET:H	1:E:319:GLN:NE2	2.13	0.41
1:C:65:LEU:CD1	1:C:118:MET:HE1	2.50	0.41
1:A:141:ASN:C	1:A:141:ASN:HD22	2.28	0.41
1:C:390:HIS:CD2	1:C:392:ASP:H	2.32	0.41
1:D:82:MET:HE1	1:D:142:HIS:NE2	2.36	0.41
1:D:344:ILE:HD11	1:D:357:TYR:CB	2.48	0.41
1:B:97:VAL:HG21	1:B:174:TRP:CH2	2.55	0.41
1:B:285:MET:HE2	1:B:378:ALA:C	2.46	0.41
1:C:80:SER:HB2	1:C:126:GLU:HA	2.02	0.41
1:C:129:MET:HE3	1:C:129:MET:HB2	1.96	0.41
1:D:92:ARG:HG3	1:D:239:TRP:NE1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLY:HA3	1:D:284:VAL:O	2.20	0.41
1:C:99:THR:HB	1:C:102:ASP:HB2	2.03	0.41
1:C:344:ILE:HG13	1:C:357:TYR:HB3	2.03	0.41
1:E:100:HIS:HD2	4:E:663:HOH:O	2.03	0.41
1:E:286:PRO:HB2	1:E:288:ASP:O	2.20	0.41
1:B:281:GLY:C	1:B:373:TRP:HB2	2.45	0.41
1:A:329:LEU:CD1	1:F:172:MET:HE1	2.52	0.40
1:C:270:SER:OG	1:C:271:ASP:N	2.54	0.40
1:D:317:GLN:HB3	1:D:318:PRO:HD2	2.02	0.40
1:F:189:PRO:HA	1:F:190:PRO:HD3	1.95	0.40
1:F:219:LEU:HD23	1:F:245:TYR:HB2	2.01	0.40
1:F:129:MET:HE2	1:F:129:MET:HB2	1.91	0.40
1:A:357:TYR:OH	1:A:377:LYS:HD3	2.22	0.40
1:E:62:TYR:OH	1:E:84:THR:OG1	2.27	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	360/401 (90%)	342 (95%)	16 (4%)	2 (1%)	21	24
1	B	341/401 (85%)	333 (98%)	8 (2%)	0	100	100
1	C	348/401 (87%)	338 (97%)	10 (3%)	0	100	100
1	D	359/401 (90%)	347 (97%)	12 (3%)	0	100	100
1	E	345/401 (86%)	336 (97%)	9 (3%)	0	100	100
1	F	373/401 (93%)	367 (98%)	6 (2%)	0	100	100
All	All	2126/2406 (88%)	2063 (97%)	61 (3%)	2 (0%)	100	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339[A]	ASP
1	A	339[B]	ASP

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	288/346 (83%)	284 (99%)	4 (1%)	59	73
1	B	284/346 (82%)	283 (100%)	1 (0%)	84	91
1	C	274/346 (79%)	269 (98%)	5 (2%)	51	66
1	D	278/346 (80%)	270 (97%)	8 (3%)	37	49
1	E	284/346 (82%)	283 (100%)	1 (0%)	84	91
1	F	306/346 (88%)	303 (99%)	3 (1%)	68	81
All	All	1714/2076 (83%)	1692 (99%)	22 (1%)	61	76

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	118	MET
1	A	275	SER
1	A	385	MET
1	B	372	ILE
1	C	84	THR
1	C	118	MET
1	C	344	ILE
1	C	355	GLU
1	C	398	ILE
1	D	208	SER
1	D	265	THR
1	D	338	ASP
1	D	344	ILE
1	D	351	GLN
1	D	394	LEU
1	D	399	LYS

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Mol	Chain	Res	Type
1	D	401	LYS
1	E	127	GLU
1	F	124	VAL
1	F	137	ASP
1	F	282	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	141	ASN
1	A	165	GLN
1	A	170	ASN
1	A	343	GLN
1	B	87	ASN
1	B	107	GLN
1	B	183	GLN
1	B	236	GLN
1	B	241	HIS
1	B	354	ASN
1	B	361	ASN
1	C	42	ASN
1	C	87	ASN
1	C	141	ASN
1	C	182	HIS
1	C	183	GLN
1	C	225	HIS
1	C	258	ASN
1	C	343	GLN
1	C	390	HIS
1	D	238	ASN
1	D	343	GLN
1	E	42	ASN
1	E	49	ASN
1	E	107	GLN
1	E	141	ASN
1	E	169	ASN
1	E	236	GLN
1	E	317	GLN
1	E	319	GLN
1	E	366	ASN
1	E	370	ASN

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Mol	Chain	Res	Type
1	F	42	ASN
1	F	49	ASN
1	F	141	ASN
1	F	241	HIS
1	F	319	GLN
1	F	324	GLN
1	F	354	ASN
1	F	370	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](#)

Of 17 ligands modelled in this entry, 11 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	T1O	E	503	1	21,21,21	6.04	13 (61%)	28,28,28	3.94	15 (53%)
3	T1O	F	503	1	21,21,21	6.11	13 (61%)	28,28,28	2.69	9 (32%)
3	T1O	D	503	1	21,21,21	6.09	13 (61%)	28,28,28	2.62	12 (42%)
3	T1O	B	502	1	21,21,21	6.03	13 (61%)	28,28,28	3.66	16 (57%)
3	T1O	A	503	1	21,21,21	6.12	13 (61%)	28,28,28	2.78	9 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	T1O	C	503	1	21,21,21	6.04	12 (57%)	28,28,28	3.03	11 (39%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T1O	E	503	1	-	7/12/33/33	0/2/2/2
3	T1O	F	503	1	-	8/12/33/33	0/2/2/2
3	T1O	D	503	1	-	6/12/33/33	0/2/2/2
3	T1O	B	502	1	-	6/12/33/33	0/2/2/2
3	T1O	A	503	1	-	9/12/33/33	0/2/2/2
3	T1O	C	503	1	-	7/12/33/33	0/2/2/2

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	T1O	C02-N08	14.11	1.61	1.35
3	D	503	T1O	C02-N08	14.03	1.61	1.35
3	C	503	T1O	C02-N08	14.00	1.61	1.35
3	A	503	T1O	C02-N08	13.96	1.60	1.35
3	F	503	T1O	C02-N08	13.81	1.60	1.35
3	B	502	T1O	C02-N08	13.78	1.60	1.35
3	E	503	T1O	C05-N08	-12.55	1.27	1.46
3	A	503	T1O	C05-N08	-12.43	1.27	1.46
3	B	502	T1O	C05-N08	-12.41	1.27	1.46
3	D	503	T1O	C05-N08	-12.37	1.27	1.46
3	C	503	T1O	C05-N08	-12.34	1.27	1.46
3	F	503	T1O	C05-N08	-12.21	1.28	1.46
3	B	502	T1O	C06-S07	-12.19	1.47	1.81
3	C	503	T1O	C06-S07	-12.15	1.47	1.81
3	E	503	T1O	C06-S07	-12.11	1.47	1.81
3	D	503	T1O	C06-S07	-12.09	1.47	1.81
3	A	503	T1O	C06-S07	-12.07	1.47	1.81
3	F	503	T1O	C06-S07	-12.07	1.47	1.81
3	D	503	T1O	C02-N03	8.68	1.51	1.35
3	F	503	T1O	C02-N03	8.62	1.51	1.35
3	C	503	T1O	C02-N03	8.27	1.50	1.35
3	B	502	T1O	C02-N03	8.26	1.50	1.35
3	A	503	T1O	C02-N03	8.10	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	T1O	C02-N03	7.80	1.49	1.35
3	F	503	T1O	C06-C05	7.70	1.69	1.53
3	B	502	T1O	C06-C05	7.68	1.69	1.53
3	D	503	T1O	C06-C05	7.67	1.69	1.53
3	A	503	T1O	C06-C05	7.60	1.69	1.53
3	C	503	T1O	C06-C05	7.58	1.69	1.53
3	E	503	T1O	C06-C05	7.46	1.68	1.53
3	F	503	T1O	C14-N15	7.13	1.50	1.33
3	A	503	T1O	C14-N15	6.84	1.49	1.33
3	D	503	T1O	C14-N15	6.23	1.48	1.33
3	E	503	T1O	C04-N03	-6.11	1.34	1.45
3	A	503	T1O	C04-N03	-6.09	1.34	1.45
3	C	503	T1O	C14-N15	6.09	1.47	1.33
3	B	502	T1O	C04-N03	-5.99	1.34	1.45
3	D	503	T1O	C04-N03	-5.91	1.34	1.45
3	F	503	T1O	C04-N03	-5.85	1.35	1.45
3	C	503	T1O	C04-N03	-5.84	1.35	1.45
3	B	502	T1O	C14-N15	5.72	1.47	1.33
3	E	503	T1O	C14-N15	5.61	1.46	1.33
3	D	503	T1O	C05-C04	4.80	1.69	1.55
3	F	503	T1O	C05-C04	4.76	1.69	1.55
3	C	503	T1O	C05-C04	4.69	1.69	1.55
3	A	503	T1O	C05-C04	4.67	1.69	1.55
3	B	502	T1O	C05-C04	4.49	1.68	1.55
3	E	503	T1O	C05-C04	4.45	1.68	1.55
3	D	503	T1O	C09-S07	-4.02	1.76	1.82
3	A	503	T1O	C09-S07	-4.01	1.76	1.82
3	F	503	T1O	C09-S07	-3.91	1.76	1.82
3	C	503	T1O	C09-S07	-3.88	1.76	1.82
3	B	502	T1O	C09-S07	-3.85	1.76	1.82
3	E	503	T1O	C09-S07	-3.82	1.76	1.82
3	A	503	T1O	C16-C17	3.21	1.56	1.51
3	A	503	T1O	C10-C09	3.02	1.60	1.52
3	D	503	T1O	C10-C09	3.00	1.60	1.52
3	F	503	T1O	C16-C17	2.92	1.55	1.51
3	B	502	T1O	C09-C04	-2.91	1.45	1.53
3	E	503	T1O	C09-C04	-2.82	1.46	1.53
3	E	503	T1O	C16-C17	2.79	1.55	1.51
3	B	502	T1O	C16-C17	2.79	1.55	1.51
3	F	503	T1O	C13-C14	2.76	1.56	1.51
3	C	503	T1O	C10-C09	2.75	1.59	1.52
3	F	503	T1O	C10-C09	2.75	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	503	T1O	C10-C09	2.73	1.59	1.52
3	C	503	T1O	C09-C04	-2.60	1.46	1.53
3	A	503	T1O	C13-C14	2.59	1.56	1.51
3	E	503	T1O	O20-C14	-2.55	1.18	1.23
3	A	503	T1O	C09-C04	-2.53	1.46	1.53
3	B	502	T1O	O20-C14	-2.52	1.18	1.23
3	B	502	T1O	C10-C09	2.49	1.59	1.52
3	F	503	T1O	C09-C04	-2.47	1.47	1.53
3	D	503	T1O	C09-C04	-2.44	1.47	1.53
3	C	503	T1O	C16-C17	2.35	1.55	1.51
3	D	503	T1O	C13-C14	2.19	1.55	1.51
3	D	503	T1O	O20-C14	-2.02	1.19	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	T1O	C17-C16-N15	-9.97	95.70	112.13
3	E	503	T1O	C06-S07-C09	8.92	108.53	89.98
3	B	502	T1O	C17-C16-N15	-8.83	97.57	112.13
3	C	503	T1O	C06-S07-C09	8.63	107.93	89.98
3	E	503	T1O	C09-C04-N03	-8.47	104.37	113.34
3	F	503	T1O	C06-S07-C09	8.43	107.52	89.98
3	B	502	T1O	C06-S07-C09	7.83	106.27	89.98
3	A	503	T1O	C06-S07-C09	7.74	106.07	89.98
3	D	503	T1O	C06-S07-C09	6.73	103.98	89.98
3	B	502	T1O	C09-C04-N03	-6.32	106.65	113.34
3	E	503	T1O	C05-C04-N03	6.08	109.54	102.68
3	A	503	T1O	C09-C04-N03	-5.59	107.43	113.34
3	D	503	T1O	C04-C05-N08	5.50	108.54	102.43
3	B	502	T1O	C05-C04-N03	5.44	108.82	102.68
3	C	503	T1O	C05-C04-N03	5.36	108.73	102.68
3	F	503	T1O	C04-C05-N08	5.27	108.28	102.43
3	A	503	T1O	C05-C04-N03	5.24	108.59	102.68
3	A	503	T1O	C04-C05-N08	5.08	108.07	102.43
3	C	503	T1O	C04-C05-N08	4.99	107.97	102.43
3	E	503	T1O	C18-C17-C16	4.99	122.60	115.51
3	F	503	T1O	C05-C04-N03	4.88	108.19	102.68
3	D	503	T1O	C05-C04-N03	4.75	108.04	102.68
3	B	502	T1O	C13-C14-N15	4.68	124.88	116.34
3	B	502	T1O	C04-C05-N08	4.68	107.62	102.43
3	C	503	T1O	C17-C16-N15	-4.61	104.53	112.13
3	B	502	T1O	C18-C17-C16	4.51	121.92	115.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	503	T1O	C04-N03-C02	-4.48	107.00	112.56
3	C	503	T1O	C04-N03-C02	-4.30	107.22	112.56
3	B	502	T1O	C04-C09-S07	4.26	109.87	105.03
3	E	503	T1O	C04-C05-N08	4.22	107.11	102.43
3	C	503	T1O	C18-C17-C16	4.17	121.44	115.51
3	A	503	T1O	C04-N03-C02	-4.14	107.42	112.56
3	B	502	T1O	C04-N03-C02	-4.11	107.46	112.56
3	B	502	T1O	C12-C13-C14	-4.03	102.00	113.19
3	E	503	T1O	O19-C17-C16	-3.94	118.32	121.31
3	E	503	T1O	C04-C09-S07	3.93	109.49	105.03
3	A	503	T1O	C18-C17-C16	3.92	121.08	115.51
3	C	503	T1O	C09-C04-N03	-3.91	109.20	113.34
3	F	503	T1O	C04-N03-C02	-3.91	107.70	112.56
3	D	503	T1O	C04-N03-C02	-3.79	107.85	112.56
3	F	503	T1O	C09-C04-N03	-3.66	109.47	113.34
3	C	503	T1O	C04-C09-S07	3.59	109.11	105.03
3	D	503	T1O	C17-C16-N15	-3.57	106.25	112.13
3	E	503	T1O	C13-C14-N15	3.52	122.76	116.34
3	D	503	T1O	C13-C14-N15	3.21	122.18	116.34
3	E	503	T1O	C12-C13-C14	-3.15	104.44	113.19
3	B	502	T1O	C09-C04-C05	-3.14	105.05	108.89
3	A	503	T1O	C05-N08-C02	-3.09	107.85	112.38
3	D	503	T1O	C05-N08-C02	-3.03	107.93	112.38
3	D	503	T1O	C18-C17-C16	3.00	119.78	115.51
3	F	503	T1O	C18-C17-C16	2.98	119.75	115.51
3	C	503	T1O	C05-N08-C02	-2.97	108.01	112.38
3	D	503	T1O	C09-C04-C05	-2.93	105.31	108.89
3	F	503	T1O	C04-C09-S07	2.93	108.36	105.03
3	F	503	T1O	C05-N08-C02	-2.93	108.08	112.38
3	C	503	T1O	O19-C17-C16	-2.83	119.16	121.31
3	B	502	T1O	O20-C14-C13	-2.80	116.94	122.02
3	D	503	T1O	C09-C04-N03	-2.73	110.45	113.34
3	E	503	T1O	C05-N08-C02	-2.62	108.53	112.38
3	A	503	T1O	C09-C04-C05	-2.60	105.71	108.89
3	B	502	T1O	C05-N08-C02	-2.60	108.56	112.38
3	B	502	T1O	C11-C10-C09	-2.50	108.28	114.04
3	C	503	T1O	C12-C13-C14	-2.50	106.25	113.19
3	B	502	T1O	O20-C14-N15	-2.49	118.15	123.03
3	F	503	T1O	C13-C14-N15	2.39	120.69	116.34
3	E	503	T1O	O20-C14-N15	-2.36	118.40	123.03
3	E	503	T1O	C09-C04-C05	-2.31	106.07	108.89
3	E	503	T1O	C10-C09-C04	-2.28	108.06	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	T1O	O20-C14-N15	-2.13	118.85	123.03
3	D	503	T1O	O19-C17-C16	-2.07	119.73	121.31
3	A	503	T1O	C13-C14-N15	2.03	120.04	116.34
3	B	502	T1O	C10-C09-C04	-2.01	108.83	114.51

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	T1O	C04-C09-C10-C11
3	A	503	T1O	S07-C09-C10-C11
3	A	503	T1O	C09-C10-C11-C12
3	A	503	T1O	C17-C16-N15-C14
3	A	503	T1O	N15-C16-C17-C18
3	B	502	T1O	N15-C16-C17-C18
3	B	502	T1O	N15-C16-C17-O19
3	C	503	T1O	N15-C16-C17-C18
3	C	503	T1O	N15-C16-C17-O19
3	D	503	T1O	C04-C09-C10-C11
3	D	503	T1O	S07-C09-C10-C11
3	E	503	T1O	N15-C16-C17-C18
3	E	503	T1O	N15-C16-C17-O19
3	F	503	T1O	C04-C09-C10-C11
3	F	503	T1O	S07-C09-C10-C11
3	F	503	T1O	N15-C16-C17-C18
3	B	502	T1O	C13-C14-N15-C16
3	C	503	T1O	C13-C14-N15-C16
3	D	503	T1O	C13-C14-N15-C16
3	E	503	T1O	C13-C14-N15-C16
3	E	503	T1O	C11-C12-C13-C14
3	C	503	T1O	C11-C12-C13-C14
3	B	502	T1O	O20-C14-N15-C16
3	C	503	T1O	O20-C14-N15-C16
3	D	503	T1O	O20-C14-N15-C16
3	E	503	T1O	O20-C14-N15-C16
3	F	503	T1O	C11-C12-C13-C14
3	F	503	T1O	C12-C13-C14-O20
3	F	503	T1O	C12-C13-C14-N15
3	C	503	T1O	C09-C10-C11-C12
3	E	503	T1O	C09-C10-C11-C12
3	B	502	T1O	C10-C11-C12-C13
3	A	503	T1O	C12-C13-C14-O20

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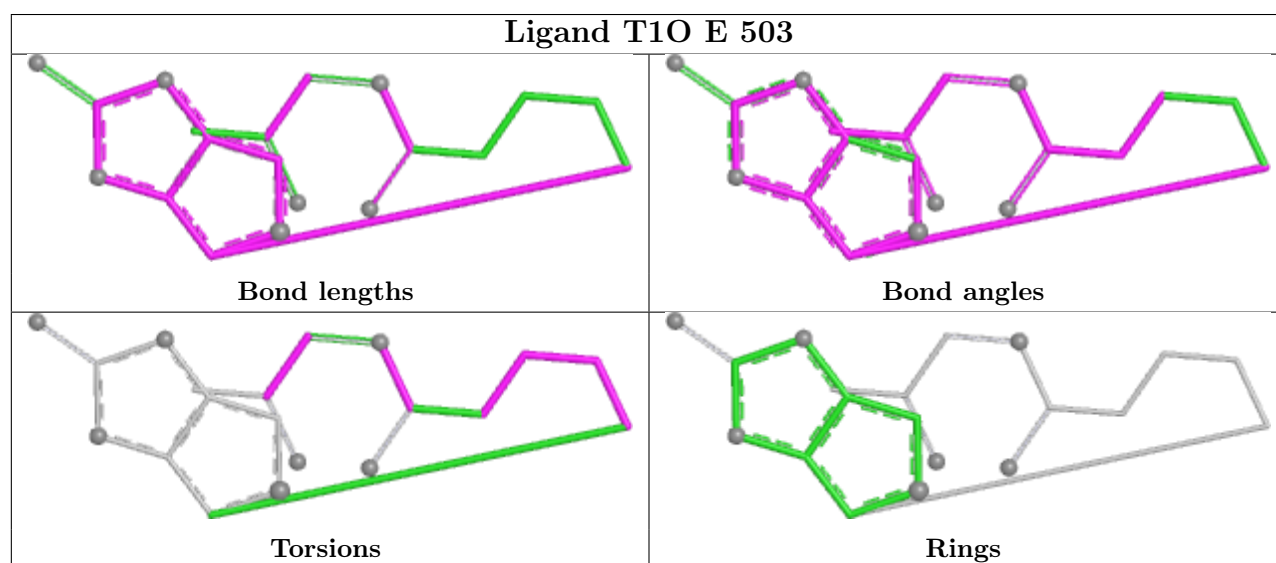
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Mol	Chain	Res	Type	Atoms
3	A	503	T1O	C10-C11-C12-C13
3	A	503	T1O	C12-C13-C14-N15
3	E	503	T1O	C10-C11-C12-C13
3	D	503	T1O	C09-C10-C11-C12
3	C	503	T1O	C10-C11-C12-C13
3	A	503	T1O	N15-C16-C17-O19
3	D	503	T1O	N15-C16-C17-O19
3	F	503	T1O	C10-C11-C12-C13
3	B	502	T1O	C09-C10-C11-C12
3	F	503	T1O	C09-C10-C11-C12

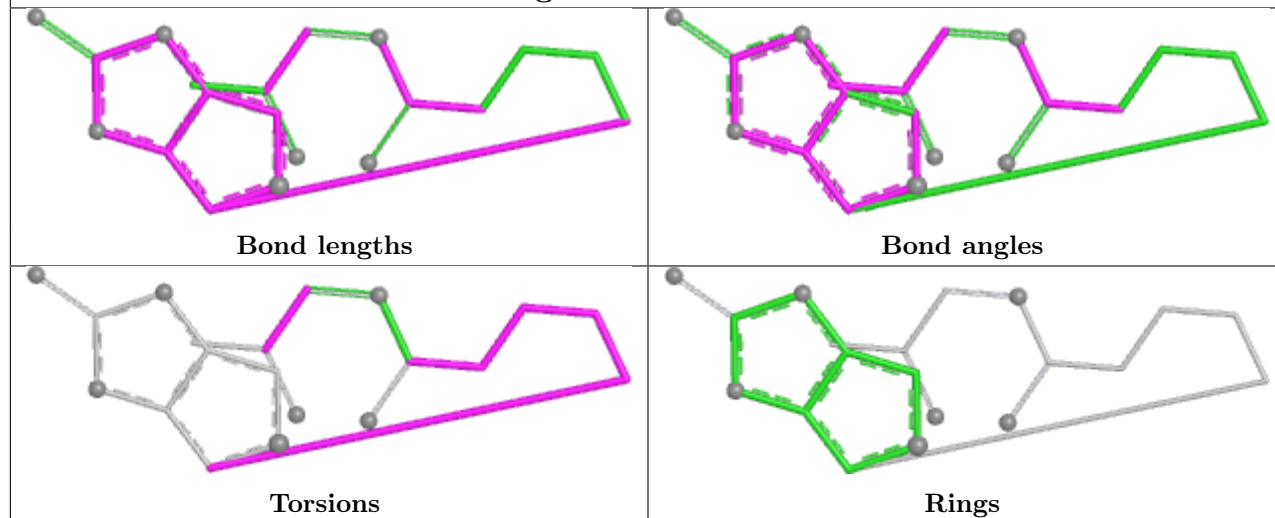
There are no ring outliers.

No monomer is involved in short contacts.

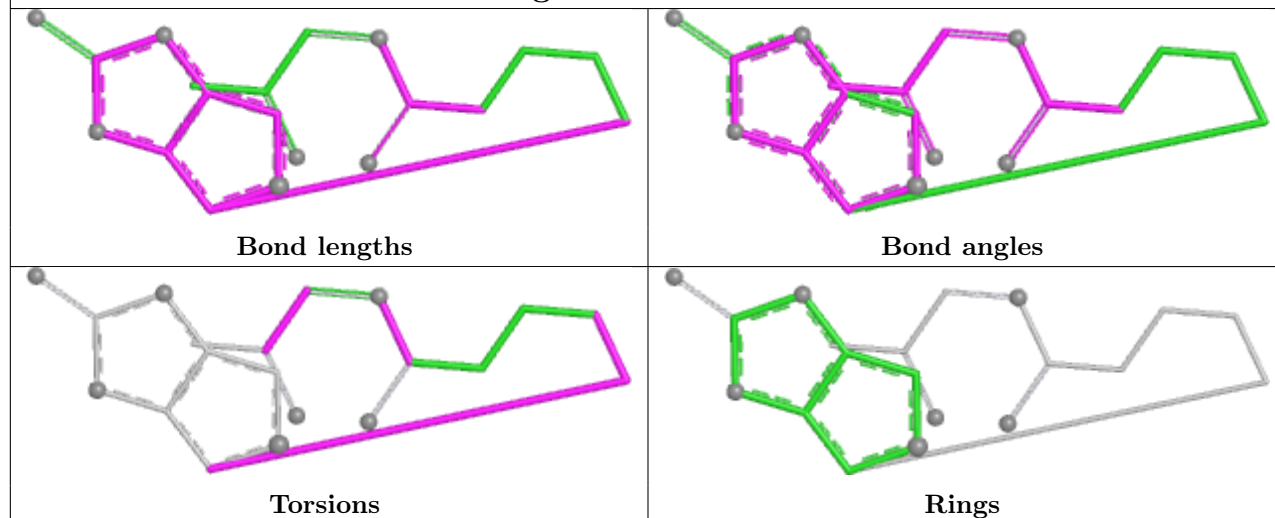
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



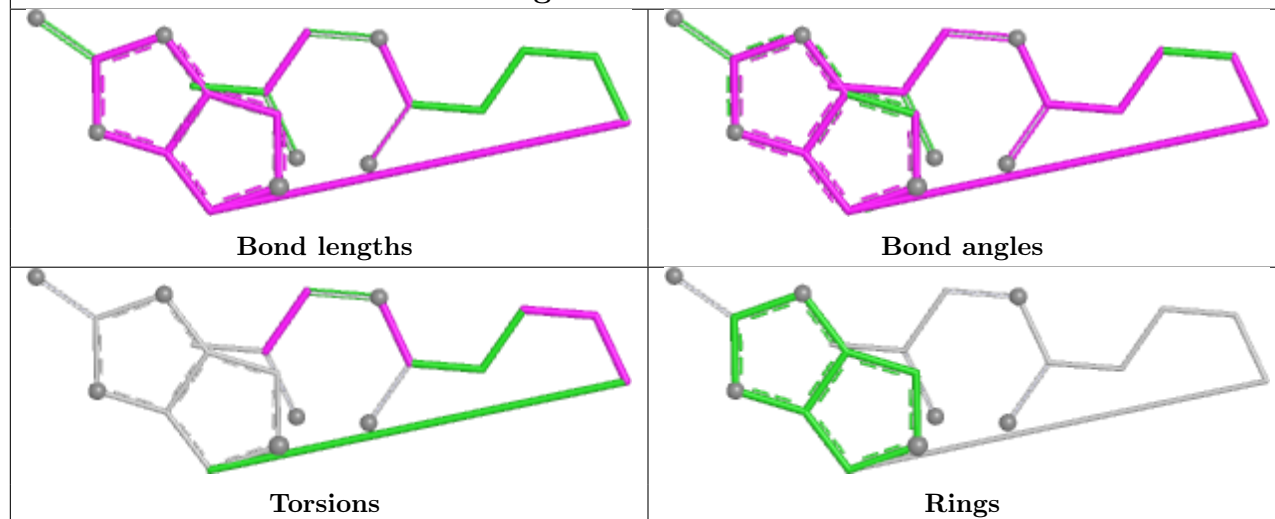
Ligand T1O F 503

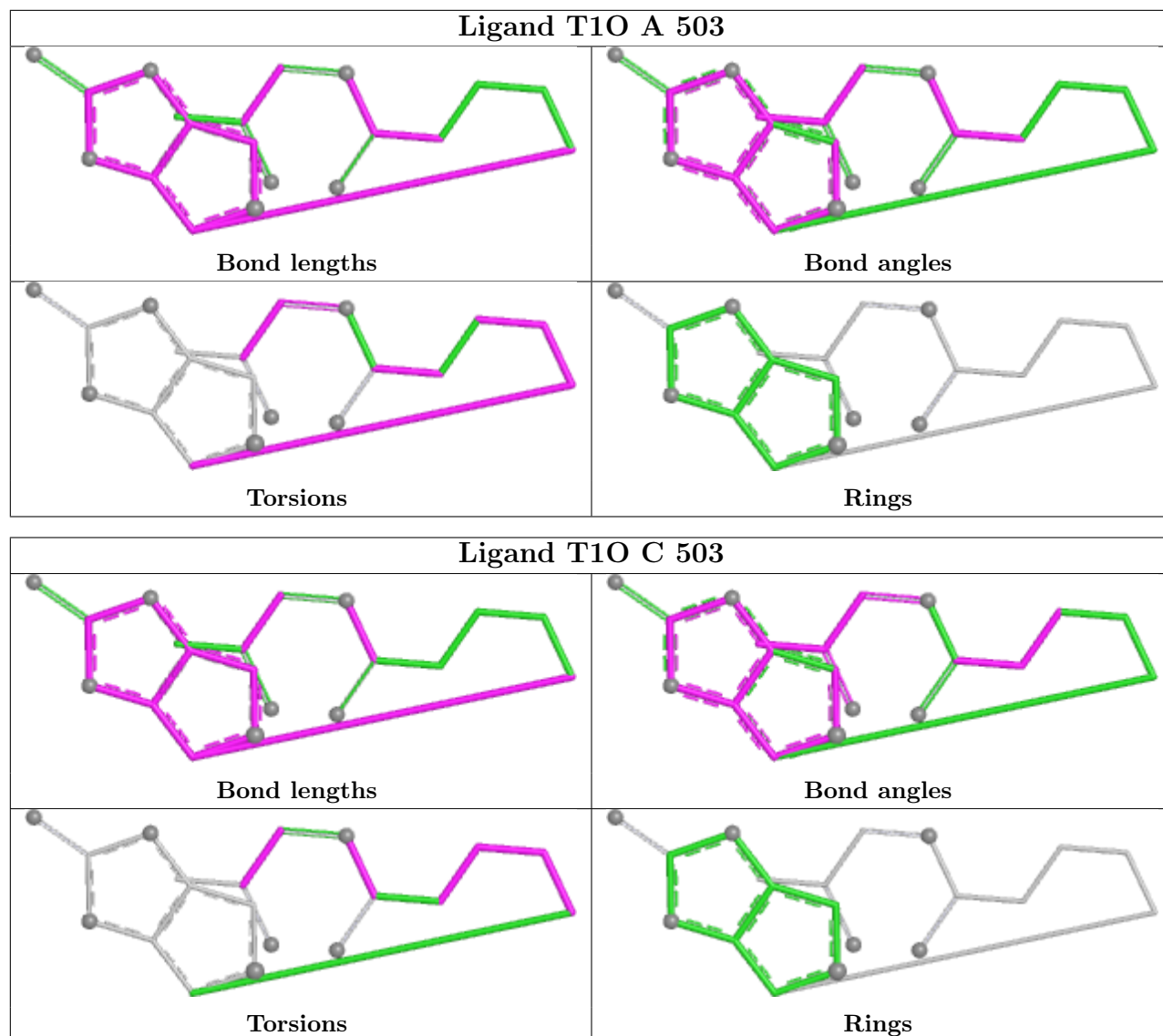


Ligand T1O D 503



Ligand T1O B 502





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	363/401 (90%)	0.29	22 (6%) 27 31	33, 60, 99, 147	1 (0%)
1	B	345/401 (86%)	0.09	11 (3%) 50 57	36, 56, 81, 116	0
1	C	352/401 (87%)	0.88	53 (15%) 5 6	42, 78, 107, 151	0
1	D	363/401 (90%)	0.60	37 (10%) 12 13	37, 72, 112, 148	0
1	E	349/401 (87%)	-0.16	12 (3%) 48 55	33, 44, 77, 125	0
1	F	374/401 (93%)	-0.24	5 (1%) 75 79	28, 42, 85, 146	1 (0%)
All	All	2146/2406 (89%)	0.24	140 (6%) 25 28	28, 56, 103, 151	2 (0%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	276	GLY	5.4
1	E	287	ASP	5.3
1	C	404	ILE	5.3
1	E	288	ASP	5.3
1	C	256	PHE	5.2
1	A	312	LEU	5.1
1	A	294	LEU	4.7
1	C	402	LEU	4.7
1	D	298	ASP	4.5
1	C	398	ILE	4.4
1	C	245	TYR	4.4
1	C	37	THR	4.2
1	F	32	GLU	3.9
1	A	295	SER	3.9
1	E	32	GLU	3.9
1	D	313	ASN	3.8
1	E	286	PRO	3.7
1	D	294	LEU	3.7
1	A	298	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	375	ALA	3.6
1	C	345	TYR	3.6
1	C	214	SER	3.6
1	C	288	ASP	3.6
1	C	374	TYR	3.5
1	D	309	GLU	3.4
1	D	288	ASP	3.4
1	B	321	TRP	3.3
1	C	378	ALA	3.2
1	C	36	PHE	3.2
1	C	321	TRP	3.2
1	D	35	VAL	3.2
1	A	299	MET	3.2
1	E	373	TRP	3.2
1	E	285	MET	3.1
1	D	33	GLY	3.1
1	C	393	ALA	3.1
1	E	314	THR	3.1
1	B	314	THR	3.0
1	D	321	TRP	3.0
1	E	280	ASP	3.0
1	F	294	LEU	3.0
1	D	295	SER	2.9
1	C	210	GLY	2.9
1	C	39	VAL	2.9
1	C	403	GLY	2.9
1	B	320	LYS	2.9
1	A	75	GLY	2.8
1	A	297	SER	2.8
1	B	373	TRP	2.8
1	D	366	ASN	2.8
1	D	292	GLN	2.8
1	D	373	TRP	2.8
1	D	297	SER	2.8
1	C	282	VAL	2.8
1	D	43	PRO	2.8
1	D	280	ASP	2.7
1	D	344	ILE	2.7
1	B	285	MET	2.7
1	F	305	LEU	2.7
1	C	357	TYR	2.7
1	A	321	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	277	PHE	2.7
1	D	37	THR	2.7
1	E	318	PRO	2.7
1	A	72	MET	2.7
1	D	283	ALA	2.6
1	A	313	ASN	2.6
1	C	227	PHE	2.6
1	C	72	MET	2.6
1	A	277	PHE	2.6
1	A	318	PRO	2.6
1	D	371	GLY	2.6
1	C	387	ILE	2.6
1	C	311	LYS	2.6
1	C	338	ASP	2.5
1	D	339	ASP	2.5
1	B	277	PHE	2.5
1	B	198	LYS	2.5
1	A	310	LYS	2.5
1	D	405	LYS	2.5
1	B	33	GLY	2.5
1	F	300	ALA	2.5
1	D	289	GLU	2.4
1	C	255	VAL	2.4
1	D	285	MET	2.4
1	C	339	ASP	2.4
1	C	358	MET	2.4
1	C	312	LEU	2.4
1	D	312	LEU	2.4
1	C	316	PRO	2.4
1	C	353	GLY	2.4
1	C	279	ARG	2.4
1	C	253	MET	2.4
1	C	344	ILE	2.4
1	C	127	GLU	2.4
1	D	345	TYR	2.3
1	B	280	ASP	2.3
1	C	373	TRP	2.3
1	D	318	PRO	2.3
1	D	374	TYR	2.3
1	C	346	GLY	2.3
1	C	314	THR	2.3
1	A	293	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	35	VAL	2.3
1	C	215	ASP	2.3
1	C	396	LYS	2.3
1	B	315	LYS	2.3
1	A	280	ASP	2.3
1	C	280	ASP	2.3
1	C	366	ASN	2.3
1	C	286	PRO	2.3
1	C	274	GLU	2.3
1	C	352	GLU	2.3
1	C	212	LYS	2.3
1	C	70	LEU	2.2
1	D	286	PRO	2.2
1	A	194	THR	2.2
1	C	64	PHE	2.2
1	D	277	PHE	2.2
1	D	364	GLY	2.2
1	C	348	ALA	2.2
1	D	265	THR	2.2
1	D	65	LEU	2.1
1	D	291	VAL	2.1
1	C	400	ALA	2.1
1	A	76	GLU	2.1
1	A	291	VAL	2.1
1	D	365	THR	2.1
1	D	311	LYS	2.1
1	B	274	GLU	2.1
1	A	292	GLN	2.1
1	D	287	ASP	2.1
1	A	286	PRO	2.1
1	E	321	TRP	2.1
1	C	395	PRO	2.0
1	C	228	TYR	2.0
1	A	296	GLY	2.0
1	C	315	LYS	2.0
1	E	274	GLU	2.0
1	F	287	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

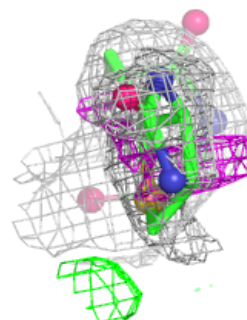
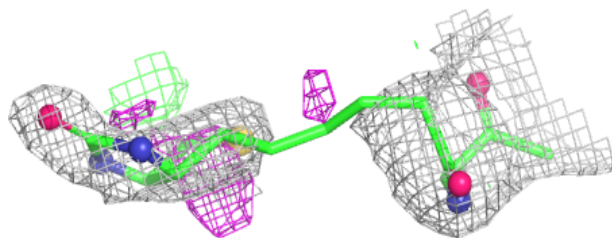
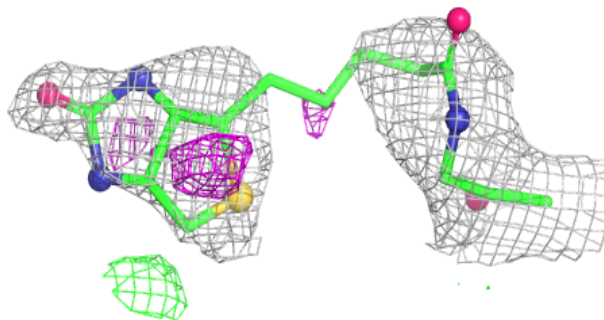
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	K	C	501	1/1	0.74	0.16	116,116,116,116	0
2	K	E	502	1/1	0.74	0.16	116,116,116,116	0
3	T1O	D	503	20/20	0.77	0.20	51,100,118,122	0
2	K	D	502	1/1	0.78	0.17	123,123,123,123	0
3	T1O	A	503	20/20	0.80	0.17	47,91,104,109	0
3	T1O	C	503	20/20	0.84	0.17	54,100,109,110	0
2	K	A	501	1/1	0.85	0.14	94,94,94,94	0
3	T1O	F	503	20/20	0.85	0.17	39,82,106,106	0
3	T1O	B	502	20/20	0.86	0.15	39,82,92,93	0
3	T1O	E	503	20/20	0.89	0.12	38,67,77,78	0
2	K	C	502	1/1	0.91	0.13	83,83,83,83	0
2	K	D	501	1/1	0.91	0.15	100,100,100,100	0
2	K	F	501	1/1	0.91	0.10	67,67,67,67	0
2	K	A	502	1/1	0.97	0.05	58,58,58,58	0
2	K	B	501	1/1	0.98	0.06	56,56,56,56	0
2	K	E	501	1/1	0.99	0.03	41,41,41,41	0
2	K	F	502	1/1	0.99	0.05	45,45,45,45	0

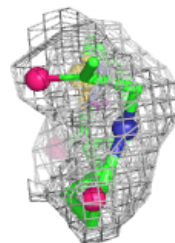
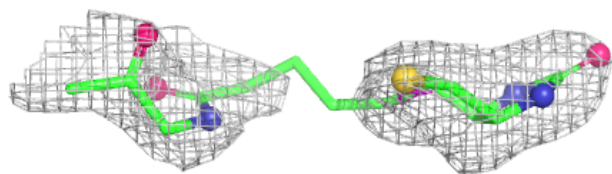
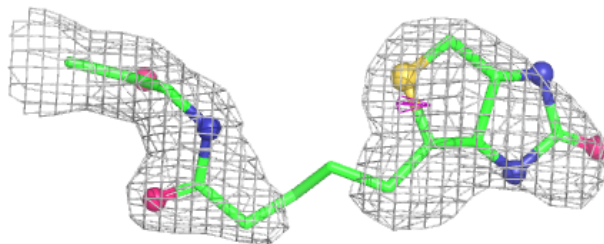
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around T1O D 503:

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

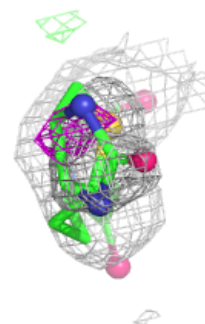
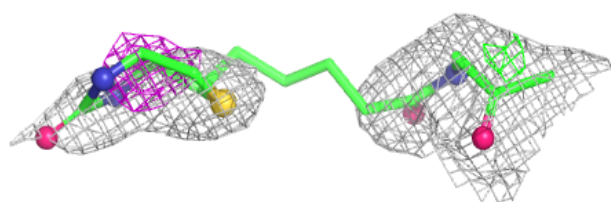
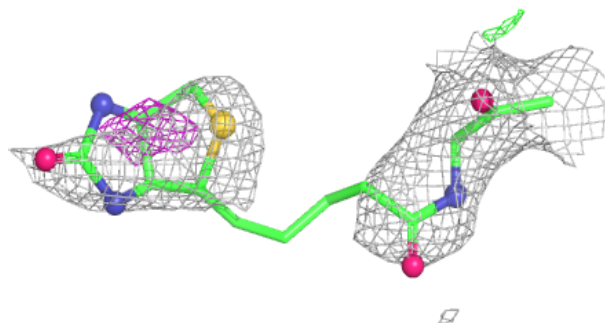
**Electron density around T1O A 503:**

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

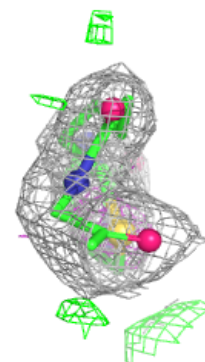
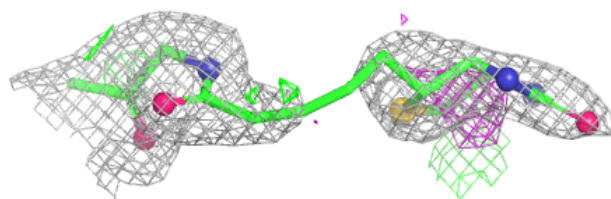
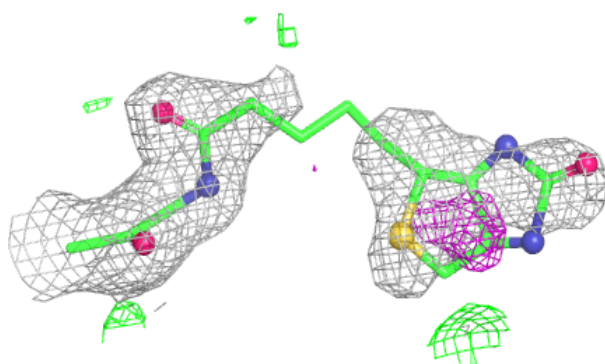


Electron density around T1O C 503:

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

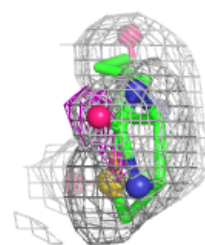
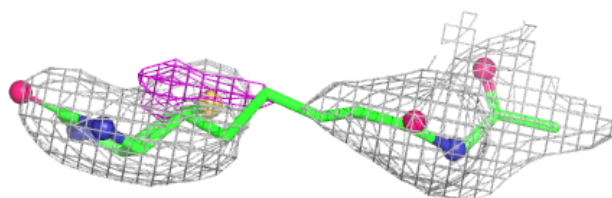
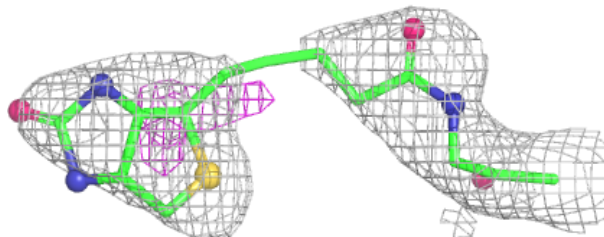
**Electron density around T1O F 503:**

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

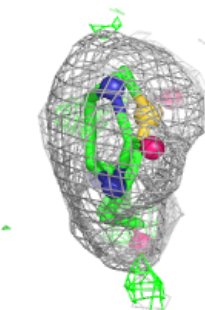
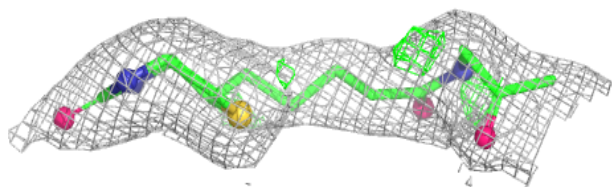
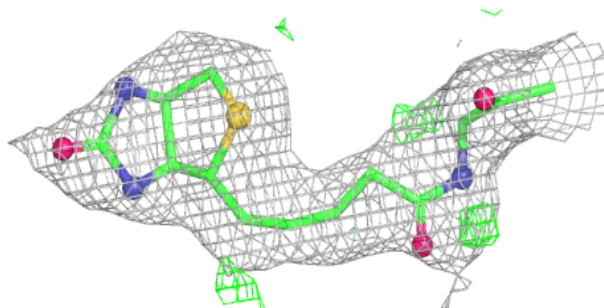


Electron density around T1O B 502:

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

**Electron density around T1O E 503:**

$2mF_o-DF_c$ (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.