



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:38 PM EDT

PDB ID : 3JPU / pdb_00003jpu
Title : LasR-TP4 complex
Authors : Zou, Y.; Nair, S.K.
Deposited on : 2009-09-04
Resolution : 2.30 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:

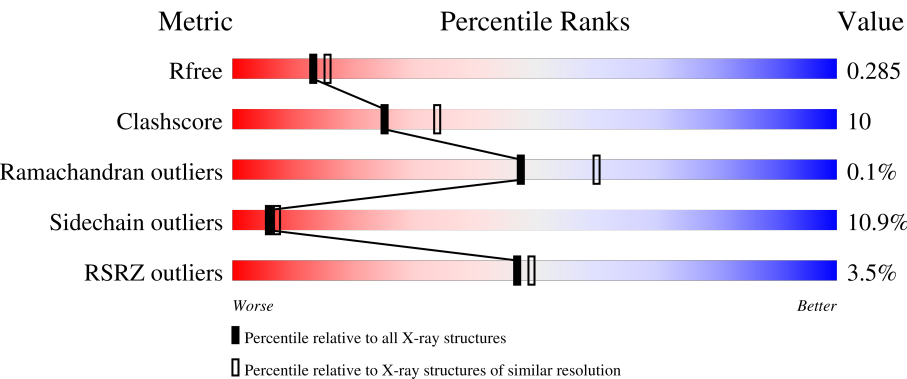
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	173	2% 65%24%5%7%
1	B	173	69%20%••7%
1	C	173	2% 73%17%•6%
1	D	173	8% 68%23%••6%
1	E	173	5% 68%21%••7%

2 Entry composition [i](#)

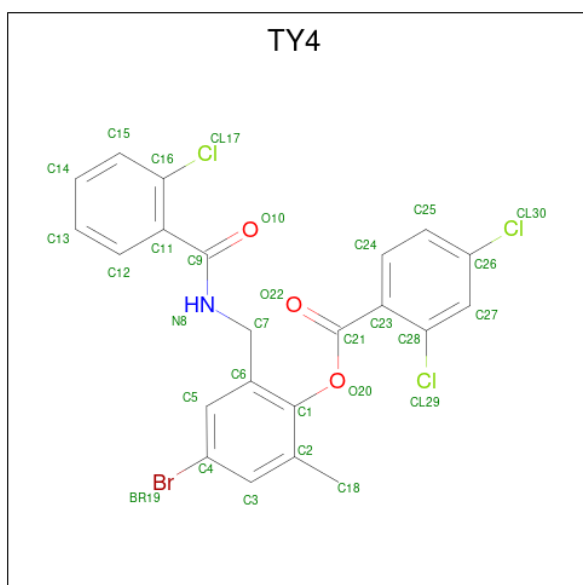
There are 3 unique types of molecules in this entry. The entry contains 6591 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional activator protein lasR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1267	812	213	237	5			
1	B	161	Total	C	N	O	S	0	0	0
			1267	812	213	237	5			
1	C	163	Total	C	N	O	S	0	0	0
			1282	821	215	241	5			
1	D	162	Total	C	N	O	S	0	0	0
			1275	816	214	240	5			
1	E	161	Total	C	N	O	S	0	0	0
			1267	812	213	237	5			

- Molecule 2 is 4-bromo-2-({[(2-chlorophenyl)carbonyl]amino}methyl)-6-methylphenyl 2,4-dichlorobenzoate (CCD ID: TY4) (formula: C₂₂H₁₅BrCl₃NO₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	0	0
			30	1	22	3	1	3		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total 30	Br 1	C 22	Cl 3	N 1	O 3	0	0
2	C	1	Total 30	Br 1	C 22	Cl 3	N 1	O 3	0	0
2	D	1	Total 30	Br 1	C 22	Cl 3	N 1	O 3	0	0
2	E	1	Total 30	Br 1	C 22	Cl 3	N 1	O 3	0	0

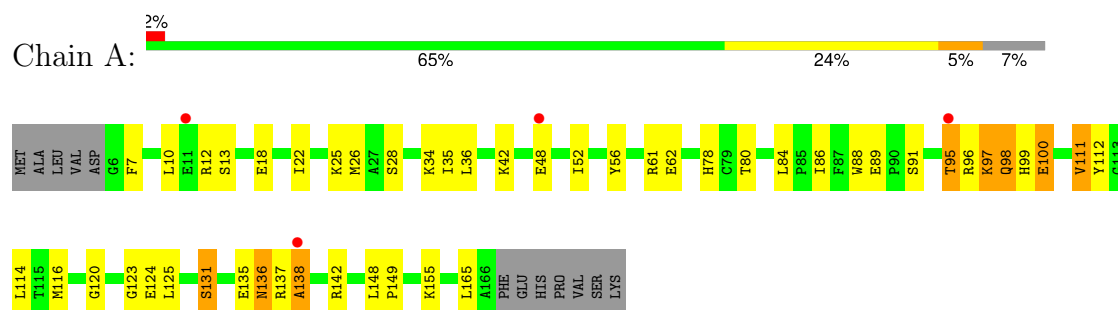
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	27	Total 27	O 27	0	0
3	C	16	Total 16	O 16	0	0
3	D	8	Total 8	O 8	0	0
3	E	12	Total 12	O 12	0	0

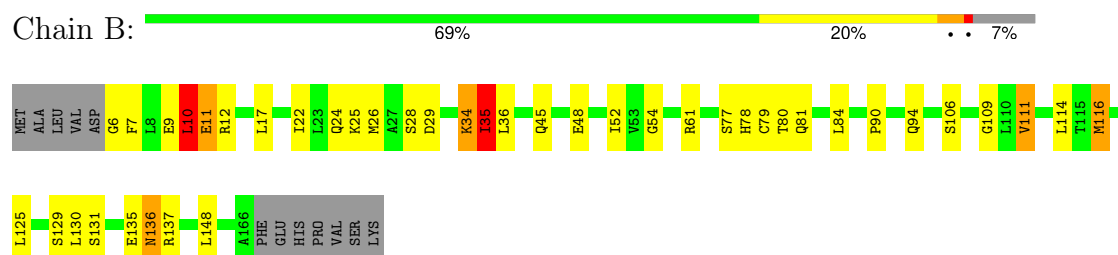
3 Residue-property plots [i](#)

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.

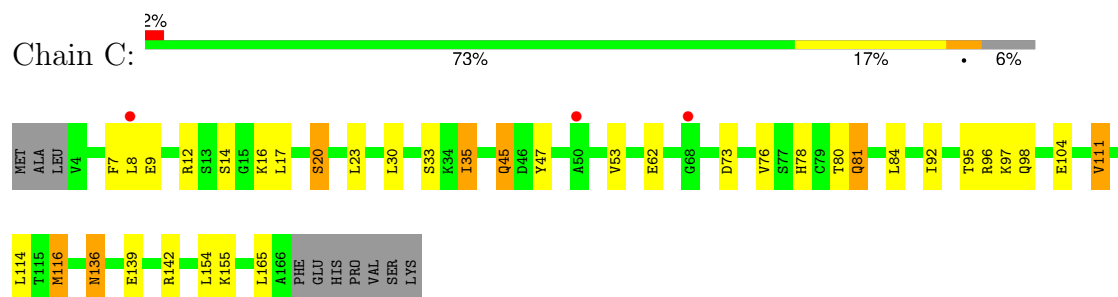
- Molecule 1: Transcriptional activator protein lasR



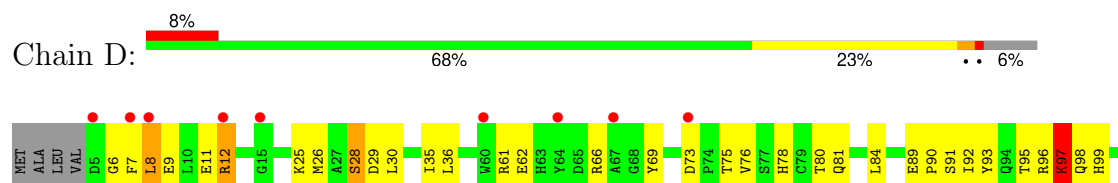
- Molecule 1: Transcriptional activator protein lasR



- Molecule 1: Transcriptional activator protein lasR



- Molecule 1: Transcriptional activator protein lasR





● Molecule 1: Transcriptional activator protein lasR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.15Å 82.43Å 90.49Å 90.00° 126.01° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (25.00-2.30) 96.1 (25.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0056	Depositor
R, R_{free}	0.225 , 0.281 0.232 , 0.285	Depositor DCC
R_{free} test set	1966 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6591	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: TY4

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	1.70	24/1300 (1.8%)	1.46	14/1761 (0.8%)
1	B	0.93	0/1300	1.17	7/1761 (0.4%)
1	C	0.87	0/1315	0.98	1/1782 (0.1%)
1	D	0.97	2/1308 (0.2%)	0.99	2/1772 (0.1%)
1	E	1.00	5/1300 (0.4%)	1.05	3/1761 (0.2%)
All	All	1.13	31/6523 (0.5%)	1.15	27/8837 (0.3%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLN	CD-NE2	15.46	1.65	1.33
1	D	97	LYS	CE-NZ	13.12	1.88	1.49
1	A	135	GLU	C-N	13.10	1.49	1.33
1	A	95	THR	C-N	12.37	1.51	1.33
1	A	136	ASN	C-O	11.70	1.35	1.23
1	E	96	ARG	NE-CZ	11.03	1.45	1.33
1	A	136	ASN	CG-OD1	10.84	1.44	1.23
1	A	135	GLU	C-O	9.98	1.38	1.24
1	A	99	HIS	CE1-NE2	9.71	1.42	1.32
1	E	96	ARG	CZ-NH1	9.64	1.46	1.32
1	E	46	ASP	C-O	8.99	1.33	1.23
1	D	97	LYS	CD-CE	8.25	1.77	1.52
1	A	97	LYS	CA-C	8.23	1.63	1.52
1	A	98	GLN	N-CA	7.75	1.56	1.46
1	A	100	GLU	CG-CD	7.49	1.70	1.52
1	A	136	ASN	CG-ND2	-7.25	1.18	1.33
1	A	99	HIS	CG-ND1	7.08	1.46	1.38
1	A	95	THR	CA-CB	6.97	1.63	1.53
1	A	138	ALA	CA-CB	6.95	1.64	1.53
1	A	99	HIS	C-N	6.62	1.42	1.33
1	A	138	ALA	CA-C	6.30	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ALA	C-O	6.12	1.31	1.24
1	A	135	GLU	CD-OE2	6.09	1.36	1.25
1	A	99	HIS	CG-CD2	6.06	1.42	1.35
1	A	138	ALA	N-CA	5.84	1.53	1.46
1	A	142	ARG	CZ-NH1	5.84	1.41	1.32
1	E	86	ILE	CA-CB	5.77	1.61	1.54
1	A	95	THR	CB-OG1	5.20	1.52	1.43
1	E	96	ARG	CD-NE	5.17	1.53	1.46
1	A	56	TYR	CA-C	-5.12	1.48	1.53
1	A	99	HIS	CA-CB	5.02	1.61	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASN	OD1-CG-ND2	-27.65	94.95	122.60
1	A	136	ASN	CA-CB-CG	9.03	121.63	112.60
1	E	96	ARG	NE-CZ-NH2	8.96	127.27	119.20
1	A	136	ASN	CB-CG-OD1	8.73	138.27	120.80
1	B	148	LEU	CA-C-N	-7.91	110.81	119.19
1	B	148	LEU	C-N-CA	-7.91	110.81	119.19
1	E	66	ARG	N-CA-C	-7.58	105.98	114.62
1	B	35	ILE	N-CA-C	7.02	117.89	108.27
1	A	111	VAL	CB-CA-C	6.92	117.60	111.71
1	A	136	ASN	CB-CA-C	-6.53	98.28	110.56
1	E	96	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
1	B	12	ARG	N-CA-C	5.95	118.49	110.88
1	A	98	GLN	OE1-CD-NE2	5.86	128.46	122.60
1	A	95	THR	CA-C-N	-5.73	112.00	121.92
1	A	95	THR	C-N-CA	-5.73	112.00	121.92
1	C	111	VAL	CB-CA-C	5.65	116.45	110.91
1	B	10	LEU	N-CA-C	-5.54	105.15	111.14
1	A	135	GLU	CB-CG-CD	-5.38	103.46	112.60
1	A	100	GLU	CB-CG-CD	-5.38	103.46	112.60
1	B	45	GLN	N-CA-C	-5.31	104.80	113.19
1	D	28	SER	N-CA-CB	5.29	117.67	110.01
1	B	111	VAL	CB-CA-C	5.22	116.40	111.44
1	A	56	TYR	CA-C-N	-5.16	114.44	119.76
1	A	56	TYR	C-N-CA	-5.16	114.44	119.76
1	A	99	HIS	CA-C-O	5.16	125.89	120.42
1	A	97	LYS	O-C-N	5.06	127.48	122.12
1	D	28	SER	CB-CA-C	-5.02	102.99	110.88

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	1267	0	1226	26	0
1	B	1267	0	1226	23	0
1	C	1282	0	1239	22	0
1	D	1275	0	1230	31	0
1	E	1267	0	1226	23	0
2	A	30	0	15	4	0
2	B	30	0	15	5	0
2	C	30	0	15	1	0
2	D	30	0	15	5	0
2	E	30	0	15	3	0
3	A	20	0	0	0	0
3	B	27	0	0	3	0
3	C	16	0	0	0	0
3	D	8	0	0	0	0
3	E	12	0	0	4	0
All	All	6591	0	6222	123	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 10.

All (123) 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:97:LYS:CD	1:D:97:LYS:CE	1.77	1.62
1:D:97:LYS:CE	1:D:97:LYS:NZ	1.88	1.36
1:B:6:GLY:HA2	3:B:176:HOH:O	1.69	0.93
1:C:73:ASP:HB3	1:C:76:VAL:HG23	1.54	0.90
1:E:75:THR:CG2	3:E:183:HOH:O	2.25	0.84
1:A:125:LEU:HG	2:A:174:TY4:CL30	2.16	0.82
1:E:75:THR:HG22	3:E:183:HOH:O	1.79	0.82
1:E:92:ILE:HD12	3:E:183:HOH:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:HIS:HE1	1:B:84:LEU:O	1.70	0.74
1:D:89:GLU:O	1:D:92:ILE:HG12	1.87	0.72
1:D:90:PRO:HA	1:D:93:TYR:HD2	1.54	0.72
1:C:73:ASP:HB3	1:C:76:VAL:CG2	2.22	0.69
1:D:97:LYS:CE	1:D:97:LYS:CG	2.69	0.69
1:D:36:LEU:CD1	1:D:61:ARG:HH21	2.05	0.68
1:D:78:HIS:HE1	1:D:84:LEU:O	1.77	0.68
1:A:42:LYS:HG3	1:A:123:GLY:HA3	1.77	0.67
1:E:39:LEU:HD11	1:E:124:GLU:HB3	1.78	0.64
1:C:23:LEU:HG	1:C:35:ILE:HD11	1.79	0.63
1:B:10:LEU:HD13	1:B:22:ILE:HG22	1.81	0.62
1:A:95:THR:OG1	1:A:98:GLN:HG3	2.01	0.61
1:B:125:LEU:HD11	2:B:174:TY4:CL30	2.37	0.61
1:B:52:ILE:HD11	2:B:174:TY4:H18B	1.81	0.60
1:C:136:ASN:HD21	1:C:139:GLU:HG3	1.67	0.59
1:E:85:PRO:HB3	1:E:116:MET:SD	2.42	0.59
1:B:135:GLU:O	1:B:136:ASN:HB3	2.02	0.59
1:D:8:LEU:O	1:D:12:ARG:HG2	2.03	0.59
1:B:34:LYS:H	1:B:131:SER:HB2	1.67	0.59
1:A:125:LEU:CG	2:A:174:TY4:CL30	2.88	0.58
1:E:42:LYS:HD3	1:E:123:GLY:HA3	1.84	0.58
1:B:90:PRO:HD3	1:B:137:ARG:NH1	2.19	0.57
1:A:61:ARG:HB3	1:A:61:ARG:NH2	2.19	0.57
1:E:33:SER:HB2	1:E:133:GLU:HG2	1.85	0.57
1:D:76:VAL:HG22	2:D:174:TY4:C24	2.34	0.57
1:C:9:GLU:OE1	1:C:9:GLU:N	2.32	0.55
1:A:52:ILE:HD11	2:A:174:TY4:H18A	1.89	0.54
1:A:112:TYR:OH	1:A:136:ASN:HA	2.08	0.54
1:C:20:SER:HB2	1:C:53:VAL:HG21	1.87	0.54
1:B:25:LYS:HE3	1:B:29:ASP:OD2	2.08	0.54
1:E:19:TRP:HH2	1:E:37:PHE:CD2	2.26	0.53
1:C:73:ASP:CB	1:C:76:VAL:HG23	2.35	0.53
1:C:165:LEU:C	1:C:165:LEU:HD12	2.34	0.52
1:D:73:ASP:OD2	2:D:174:TY4:N8	2.34	0.52
1:B:6:GLY:CA	3:B:176:HOH:O	2.42	0.51
1:C:78:HIS:HE1	1:C:84:LEU:O	1.95	0.50
1:E:92:ILE:CD1	3:E:183:HOH:O	2.51	0.50
1:C:45:GLN:HG2	1:C:47:TYR:CE2	2.47	0.49
1:D:153:MET:HE3	1:E:152:TRP:CZ3	2.47	0.49
1:E:118:LEU:HB3	1:E:159:LEU:HD22	1.95	0.49
1:A:89:GLU:HG2	1:A:137:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:O	1:A:96:ARG:HG2	2.13	0.48
1:A:36:LEU:C	1:A:36:LEU:HD23	2.39	0.48
1:B:35:ILE:HG12	1:B:36:LEU:N	2.27	0.48
1:A:116:MET:HE2	1:A:155:LYS:HG2	1.95	0.47
1:D:62:GLU:O	1:D:66:ARG:HB2	2.14	0.47
1:A:136:ASN:HD22	1:A:138:ALA:H	1.62	0.47
1:B:106:SER:O	1:B:109:GLY:N	2.37	0.47
1:E:52:ILE:HD11	2:E:174:TY4:H18A	1.96	0.47
1:A:10:LEU:HD13	1:A:22:ILE:HG22	1.96	0.47
1:C:116:MET:HE2	1:C:155:LYS:HE2	1.96	0.47
1:D:62:GLU:HA	1:D:62:GLU:OE1	2.14	0.47
1:D:75:THR:HG21	2:D:174:TY4:H12	1.96	0.47
1:A:96:ARG:O	1:A:100:GLU:HG3	2.15	0.47
1:D:96:ARG:HA	1:D:99:HIS:HB2	1.97	0.47
1:E:138:ALA:O	1:E:142:ARG:HD2	2.15	0.47
1:A:52:ILE:HD13	1:A:61:ARG:HH11	1.80	0.46
1:A:88:TRP:N	1:A:88:TRP:CD1	2.81	0.46
1:B:129:SER:C	1:B:130:LEU:HG	2.40	0.46
1:E:13:SER:HB2	1:E:18:GLU:HG2	1.96	0.46
1:A:78:HIS:HE1	1:A:84:LEU:O	1.98	0.46
1:E:41:PRO:HG2	1:E:44:SER:HB2	1.96	0.46
1:A:148:LEU:HB3	1:A:149:PRO:HD3	1.96	0.46
1:B:36:LEU:C	1:B:36:LEU:HD23	2.41	0.46
1:D:7:PHE:CD1	1:D:26:MET:HE1	2.51	0.46
1:C:16:LYS:O	1:C:20:SER:HB3	2.16	0.46
1:C:45:GLN:HG2	1:C:47:TYR:HE2	1.81	0.46
1:D:153:MET:HG2	1:E:152:TRP:CE3	2.50	0.45
1:D:97:LYS:HD3	1:D:97:LYS:H	1.80	0.45
1:A:97:LYS:HA	1:A:100:GLU:HG3	1.97	0.45
1:C:8:LEU:O	1:C:12:ARG:HG2	2.17	0.45
1:A:7:PHE:CD1	1:A:26:MET:HE1	2.52	0.45
1:C:14:SER:O	1:D:95:THR:HB	2.17	0.45
1:E:111:VAL:HG23	1:E:112:TYR:H	1.82	0.44
1:E:76:VAL:HA	2:E:174:TY4:H25	1.99	0.44
1:D:119:HIS:CE1	1:D:125:LEU:HD13	2.53	0.44
1:B:79:CYS:HB3	2:B:174:TY4:CL30	2.55	0.44
1:B:61:ARG:NH2	3:B:180:HOH:O	2.51	0.44
1:D:95:THR:OG1	1:D:98:GLN:HG3	2.17	0.44
1:E:77:SER:O	1:E:81:GLN:HG3	2.18	0.44
1:B:35:ILE:O	1:B:54:GLY:HA3	2.17	0.44
1:D:125:LEU:HD11	2:D:174:TY4:CL30	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:MET:HE2	1:B:116:MET:HB3	1.90	0.43
1:D:36:LEU:HD11	1:D:61:ARG:HH21	1.82	0.43
1:A:13:SER:HB2	1:A:18:GLU:HG2	2.00	0.43
1:C:80:THR:HG22	1:C:81:GLN:HE21	1.83	0.43
1:B:79:CYS:CB	2:B:174:TY4:CL30	3.03	0.43
1:E:40:LEU:HD13	1:E:44:SER:O	2.19	0.43
1:A:125:LEU:CD1	2:A:174:TY4:CL30	3.04	0.42
1:C:95:THR:OG1	1:C:98:GLN:HG3	2.19	0.42
1:B:52:ILE:HD11	2:B:174:TY4:C18	2.48	0.42
1:D:99:HIS:O	1:D:103:GLU:HG3	2.20	0.42
1:B:11:GLU:O	1:B:11:GLU:HG3	2.19	0.42
1:D:69:TYR:OH	1:D:104:GLU:OE1	2.33	0.42
1:E:51:PHE:CD1	1:E:166:ALA:HA	2.54	0.42
1:C:7:PHE:HE1	1:C:154:LEU:HA	1.85	0.42
1:C:136:ASN:ND2	1:C:139:GLU:H	2.17	0.42
1:D:76:VAL:HG22	2:D:174:TY4:H24	2.02	0.42
1:D:96:ARG:HG2	1:D:99:HIS:CD2	2.54	0.41
1:C:76:VAL:HA	2:C:174:TY4:H25	2.02	0.41
1:C:116:MET:CE	1:C:155:LYS:HE2	2.50	0.41
1:A:52:ILE:HG21	1:A:61:ARG:HE	1.85	0.41
1:D:6:GLY:HA2	1:D:9:GLU:OE1	2.21	0.41
1:B:77:SER:O	1:B:81:GLN:HG3	2.21	0.41
1:D:25:LYS:HE3	1:D:29:ASP:OD2	2.21	0.41
1:D:116:MET:HA	1:D:117:PRO:HD3	1.96	0.41
1:E:165:LEU:O	1:E:166:ALA:C	2.63	0.41
1:A:120:GLY:HA3	1:A:124:GLU:OE1	2.20	0.40
1:E:62:GLU:CD	1:E:66:ARG:HH12	2.29	0.40
2:E:174:TY4:O22	2:E:174:TY4:CL29	2.76	0.40
1:A:34:LYS:HB2	1:A:131:SER:HB2	2.04	0.40
1:A:112:TYR:CE1	1:A:137:ARG:HB2	2.56	0.40
1:B:7:PHE:CD1	1:B:26:MET:HE1	2.57	0.40
1:C:23:LEU:HD12	1:C:23:LEU:O	2.21	0.40
1:D:30:LEU:HD12	1:D:30:LEU:HA	1.92	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	159/173 (92%)	155 (98%)	4 (2%)	0	100	100
1	B	159/173 (92%)	155 (98%)	4 (2%)	0	100	100
1	C	161/173 (93%)	152 (94%)	9 (6%)	0	100	100
1	D	160/173 (92%)	151 (94%)	9 (6%)	0	100	100
1	E	159/173 (92%)	144 (91%)	14 (9%)	1 (1%)	21	27
All	All	798/865 (92%)	757 (95%)	40 (5%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	14	SER

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	130/141 (92%)	117 (90%)	13 (10%)	7	9
1	B	130/141 (92%)	115 (88%)	15 (12%)	5	6
1	C	132/141 (94%)	115 (87%)	17 (13%)	4	4
1	D	131/141 (93%)	117 (89%)	14 (11%)	6	8
1	E	130/141 (92%)	118 (91%)	12 (9%)	8	11
All	All	653/705 (93%)	582 (89%)	71 (11%)	6	7

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	25	LYS
1	A	28	SER
1	A	35	ILE
1	A	48	GLU
1	A	62	GLU
1	A	80	THR
1	A	86	ILE
1	A	91	SER
1	A	111	VAL
1	A	114	LEU
1	A	131	SER
1	A	165	LEU
1	B	9	GLU
1	B	10	LEU
1	B	11	GLU
1	B	17	LEU
1	B	24	GLN
1	B	28	SER
1	B	34	LYS
1	B	35	ILE
1	B	48	GLU
1	B	80	THR
1	B	94	GLN
1	B	111	VAL
1	B	114	LEU
1	B	116	MET
1	B	136	ASN
1	C	17	LEU
1	C	20	SER
1	C	30	LEU
1	C	33	SER
1	C	35	ILE
1	C	45	GLN
1	C	62	GLU
1	C	81	GLN
1	C	92	ILE
1	C	96	ARG
1	C	97	LYS
1	C	104	GLU
1	C	111	VAL
1	C	114	LEU

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Mol	Chain	Res	Type
1	C	116	MET
1	C	136	ASN
1	C	142	ARG
1	D	8	LEU
1	D	11	GLU
1	D	12	ARG
1	D	28	SER
1	D	35	ILE
1	D	80	THR
1	D	81	GLN
1	D	91	SER
1	D	97	LYS
1	D	111	VAL
1	D	114	LEU
1	D	116	MET
1	D	122	ARG
1	D	165	LEU
1	E	11	GLU
1	E	30	LEU
1	E	35	ILE
1	E	66	ARG
1	E	89	GLU
1	E	92	ILE
1	E	96	ARG
1	E	100	GLU
1	E	111	VAL
1	E	114	LEU
1	E	152	TRP
1	E	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	78	HIS
1	A	81	GLN
1	A	136	ASN
1	B	49	ASN
1	B	78	HIS
1	C	63	HIS
1	C	78	HIS
1	C	81	GLN

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Mol	Chain	Res	Type
1	C	136	ASN
1	D	49	ASN
1	D	78	HIS
1	D	81	GLN
1	D	136	ASN
1	E	78	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 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	TY4	A	174	-	32,32,32	2.12	8 (25%)	45,45,45	2.17	18 (40%)
2	TY4	C	174	-	32,32,32	2.35	7 (21%)	45,45,45	1.90	14 (31%)
2	TY4	B	174	-	32,32,32	2.48	8 (25%)	45,45,45	2.41	18 (40%)
2	TY4	E	174	-	32,32,32	2.65	9 (28%)	45,45,45	1.71	9 (20%)
2	TY4	D	174	-	32,32,32	2.35	9 (28%)	45,45,45	1.92	15 (33%)

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	TY4	A	174	-	-	4/17/17/17	0/3/3/3
2	TY4	C	174	-	-	4/17/17/17	0/3/3/3
2	TY4	B	174	-	-	5/17/17/17	0/3/3/3
2	TY4	E	174	-	-	5/17/17/17	0/3/3/3
2	TY4	D	174	-	-	3/17/17/17	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	174	TY4	C11-C16	7.89	1.50	1.39
2	C	174	TY4	C11-C16	7.23	1.49	1.39
2	D	174	TY4	C11-C16	6.75	1.49	1.39
2	B	174	TY4	C11-C16	6.74	1.49	1.39
2	B	174	TY4	C23-C28	6.57	1.48	1.39
2	A	174	TY4	C11-C16	6.56	1.48	1.39
2	E	174	TY4	C1-C2	6.45	1.51	1.40
2	C	174	TY4	C23-C28	6.09	1.48	1.39
2	B	174	TY4	C1-C2	5.95	1.50	1.40
2	E	174	TY4	C23-C28	5.89	1.47	1.39
2	D	174	TY4	C23-C28	5.14	1.46	1.39
2	E	174	TY4	C1-C6	5.14	1.49	1.40
2	D	174	TY4	C1-C2	4.89	1.48	1.40
2	A	174	TY4	C23-C28	4.81	1.46	1.39
2	D	174	TY4	C1-C6	4.74	1.48	1.40
2	A	174	TY4	C1-C2	4.61	1.48	1.40
2	C	174	TY4	C1-C2	4.51	1.48	1.40
2	C	174	TY4	C16-CL17	4.09	1.83	1.73
2	D	174	TY4	C16-CL17	4.09	1.83	1.73
2	C	174	TY4	C1-C6	4.02	1.47	1.40
2	B	174	TY4	C16-CL17	3.40	1.81	1.73
2	B	174	TY4	C1-C6	3.34	1.46	1.40
2	E	174	TY4	C16-CL17	3.30	1.81	1.73
2	A	174	TY4	O20-C1	-3.18	1.34	1.40
2	B	174	TY4	O20-C21	3.06	1.45	1.35
2	E	174	TY4	O20-C1	-2.95	1.35	1.40
2	C	174	TY4	O20-C1	-2.94	1.35	1.40
2	D	174	TY4	C28-CL29	2.91	1.80	1.73
2	B	174	TY4	O20-C1	-2.83	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	174	TY4	O20-C21	2.77	1.44	1.35
2	D	174	TY4	O20-C1	-2.71	1.35	1.40
2	E	174	TY4	C26-CL30	2.58	1.80	1.74
2	E	174	TY4	C28-CL29	2.55	1.79	1.73
2	A	174	TY4	C16-CL17	2.55	1.79	1.73
2	A	174	TY4	O20-C21	2.45	1.43	1.35
2	C	174	TY4	O20-C21	2.37	1.43	1.35
2	B	174	TY4	C26-CL30	2.35	1.79	1.74
2	A	174	TY4	C1-C6	2.31	1.44	1.40
2	D	174	TY4	C26-CL30	2.25	1.79	1.74
2	A	174	TY4	BR19-C4	-2.04	1.86	1.90
2	D	174	TY4	O20-C21	2.03	1.42	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	174	TY4	C27-C26-CL30	-6.27	111.30	119.17
2	B	174	TY4	C25-C26-CL30	-5.28	111.56	119.36
2	B	174	TY4	BR19-C4-C5	-5.19	111.90	119.23
2	B	174	TY4	C23-C28-CL29	-4.82	113.90	121.01
2	A	174	TY4	BR19-C4-C5	-4.80	112.45	119.23
2	B	174	TY4	C27-C28-CL29	4.60	125.98	118.45
2	A	174	TY4	C5-C4-C3	4.34	127.70	121.53
2	B	174	TY4	C27-C26-CL30	4.33	124.60	119.17
2	D	174	TY4	C27-C28-C23	-4.24	118.12	121.59
2	C	174	TY4	O10-C9-C11	-3.90	113.89	121.03
2	C	174	TY4	C11-C9-N8	3.80	124.71	117.32
2	D	174	TY4	C24-C23-C28	3.78	122.21	117.79
2	E	174	TY4	C27-C28-C23	-3.76	118.51	121.59
2	C	174	TY4	C25-C26-CL30	-3.70	113.90	119.36
2	B	174	TY4	O20-C1-C2	3.58	123.67	117.93
2	E	174	TY4	BR19-C4-C3	-3.56	114.19	119.23
2	E	174	TY4	C24-C23-C28	3.48	121.86	117.79
2	D	174	TY4	C16-C11-C9	-3.42	117.02	122.56
2	C	174	TY4	C15-C16-C11	-3.42	117.57	121.36
2	C	174	TY4	C24-C23-C28	3.35	121.71	117.79
2	E	174	TY4	C27-C28-CL29	3.30	123.85	118.45
2	B	174	TY4	C11-C9-N8	3.29	123.72	117.32
2	E	174	TY4	C5-C4-C3	3.26	126.17	121.53
2	B	174	TY4	C24-C23-C28	3.26	121.61	117.79
2	C	174	TY4	C28-C27-C26	-3.23	115.08	118.72
2	A	174	TY4	C25-C26-CL30	3.18	124.05	119.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	174	TY4	C18-C2-C1	3.16	125.87	120.80
2	C	174	TY4	C25-C26-C27	3.12	125.62	121.53
2	D	174	TY4	C11-C9-N8	3.10	123.35	117.32
2	D	174	TY4	C27-C28-CL29	3.07	123.48	118.45
2	D	174	TY4	C15-C16-CL17	3.06	124.45	118.42
2	A	174	TY4	C28-C23-C21	-3.05	117.55	123.94
2	E	174	TY4	O20-C1-C2	3.03	122.80	117.93
2	B	174	TY4	C28-C27-C26	-3.02	115.31	118.72
2	C	174	TY4	C7-C6-C5	2.94	126.00	120.34
2	D	174	TY4	O20-C1-C2	2.87	122.54	117.93
2	B	174	TY4	C24-C25-C26	2.81	122.07	119.24
2	A	174	TY4	C12-C11-C16	-2.80	114.52	117.79
2	B	174	TY4	BR19-C4-C3	2.77	123.15	119.23
2	B	174	TY4	O10-C9-C11	-2.72	116.04	121.03
2	A	174	TY4	O20-C1-C2	2.72	122.30	117.93
2	B	174	TY4	O20-C1-C6	-2.71	113.80	118.43
2	A	174	TY4	C1-O20-C21	2.71	124.36	117.49
2	D	174	TY4	O10-C9-N8	-2.69	117.35	122.59
2	D	174	TY4	C11-C16-CL17	-2.68	117.06	121.01
2	A	174	TY4	C25-C24-C23	-2.65	116.49	120.86
2	A	174	TY4	O20-C1-C6	-2.64	113.91	118.43
2	D	174	TY4	C5-C4-C3	2.64	125.28	121.53
2	A	174	TY4	C24-C23-C28	2.63	120.87	117.79
2	D	174	TY4	C15-C16-C11	-2.62	118.46	121.36
2	D	174	TY4	C12-C11-C9	2.61	125.48	118.53
2	D	174	TY4	C28-C23-C21	-2.60	118.49	123.94
2	A	174	TY4	C6-C1-C2	2.50	123.78	120.25
2	A	174	TY4	O10-C9-N8	-2.41	117.89	122.59
2	B	174	TY4	C5-C4-C3	2.40	124.94	121.53
2	A	174	TY4	C25-C26-C27	2.35	124.61	121.53
2	C	174	TY4	C16-C11-C9	-2.35	118.76	122.56
2	D	174	TY4	C7-C6-C5	2.32	124.80	120.34
2	C	174	TY4	C27-C28-CL29	2.32	122.24	118.45
2	B	174	TY4	C25-C24-C23	-2.31	117.06	120.86
2	E	174	TY4	C23-C28-CL29	-2.29	117.63	121.01
2	A	174	TY4	C11-C16-CL17	-2.27	117.66	121.01
2	B	174	TY4	C18-C2-C3	2.22	123.48	119.57
2	B	174	TY4	C7-C6-C5	2.18	124.53	120.34
2	B	174	TY4	O22-C21-C23	2.16	128.82	121.59
2	C	174	TY4	O20-C1-C2	2.15	121.38	117.93
2	C	174	TY4	C7-N8-C9	-2.14	116.86	121.89
2	C	174	TY4	C27-C28-C23	-2.13	119.84	121.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	174	TY4	C23-C28-CL29	-2.11	117.90	121.01
2	A	174	TY4	C28-C27-C26	-2.09	116.36	118.72
2	A	174	TY4	C18-C2-C3	2.08	123.23	119.57
2	A	174	TY4	C7-C6-C5	2.02	124.22	120.34
2	D	174	TY4	C1-O20-C21	2.02	122.62	117.49
2	E	174	TY4	C15-C16-C11	-2.00	119.14	121.36

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	174	TY4	C1-C6-C7-N8
2	A	174	TY4	C1-C6-C7-N8
2	E	174	TY4	C2-C1-O20-C21
2	B	174	TY4	O20-C21-C23-C28
2	B	174	TY4	C1-C6-C7-N8
2	C	174	TY4	C1-C6-C7-N8
2	E	174	TY4	C1-C6-C7-N8
2	C	174	TY4	C5-C6-C7-N8
2	A	174	TY4	C12-C11-C9-O10
2	C	174	TY4	C12-C11-C9-O10
2	B	174	TY4	C12-C11-C9-O10
2	C	174	TY4	C12-C11-C9-N8
2	A	174	TY4	C12-C11-C9-N8
2	B	174	TY4	C5-C6-C7-N8
2	E	174	TY4	C12-C11-C9-O10
2	B	174	TY4	C12-C11-C9-N8
2	A	174	TY4	C5-C6-C7-N8
2	E	174	TY4	C6-C1-O20-C21
2	D	174	TY4	C12-C11-C9-N8
2	E	174	TY4	C12-C11-C9-N8
2	D	174	TY4	C5-C6-C7-N8

There are no ring outliers.

5 monomers are involved in 18 short contacts:

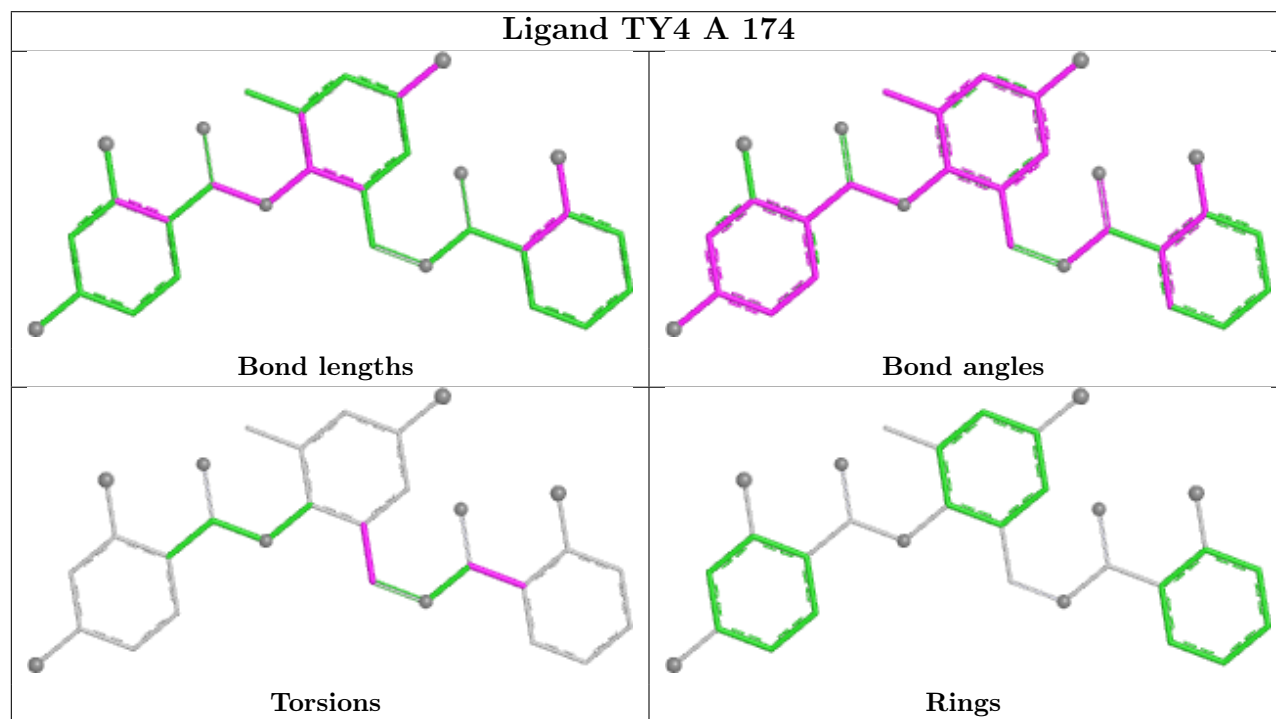
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	174	TY4	4	0
2	C	174	TY4	1	0
2	B	174	TY4	5	0
2	E	174	TY4	3	0

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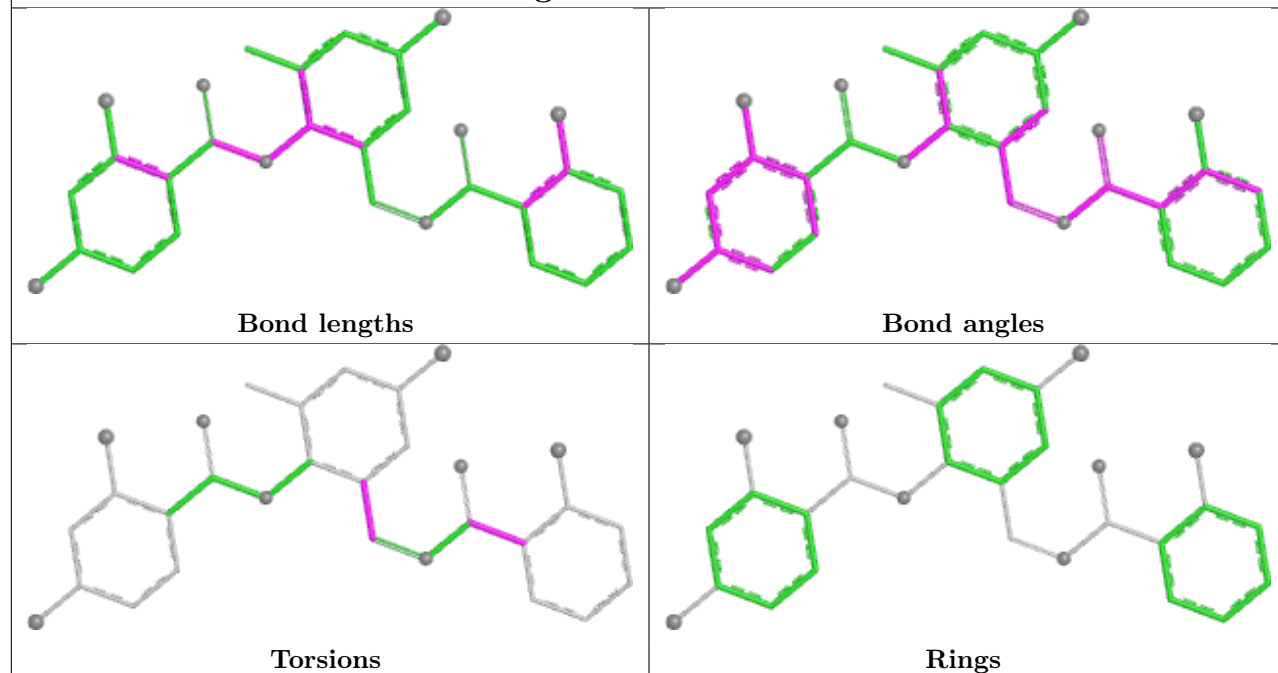
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	174	TY4	5	0

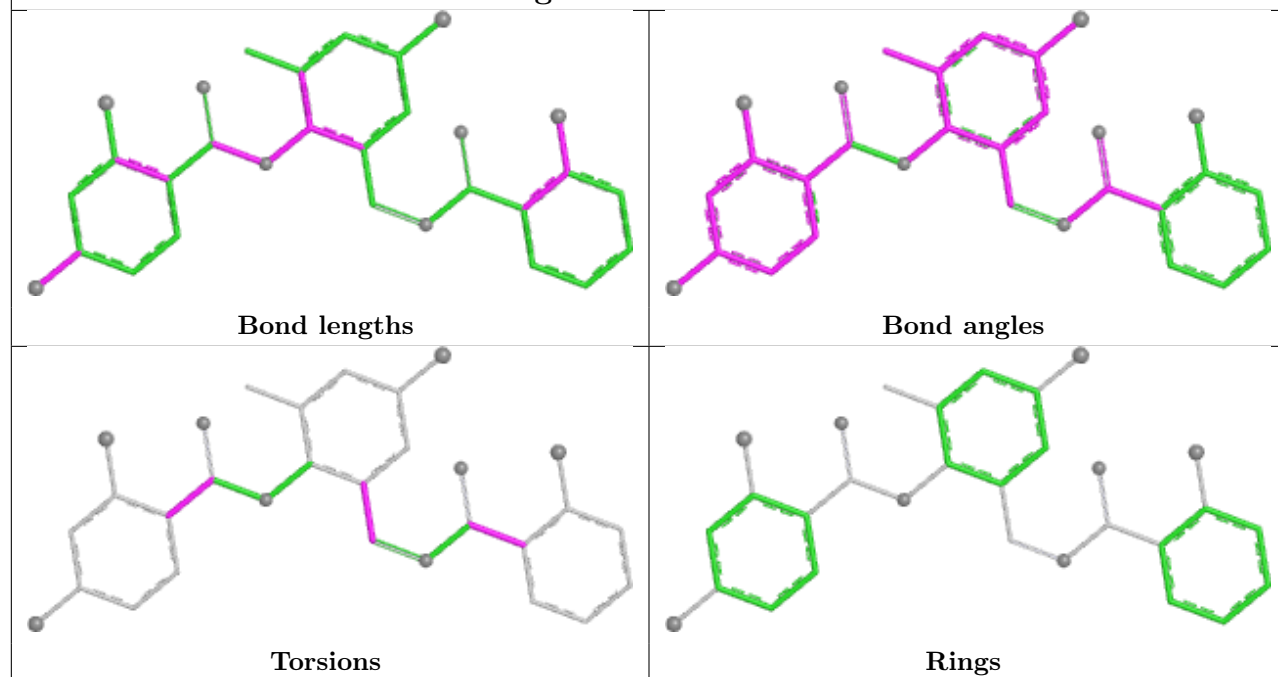
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

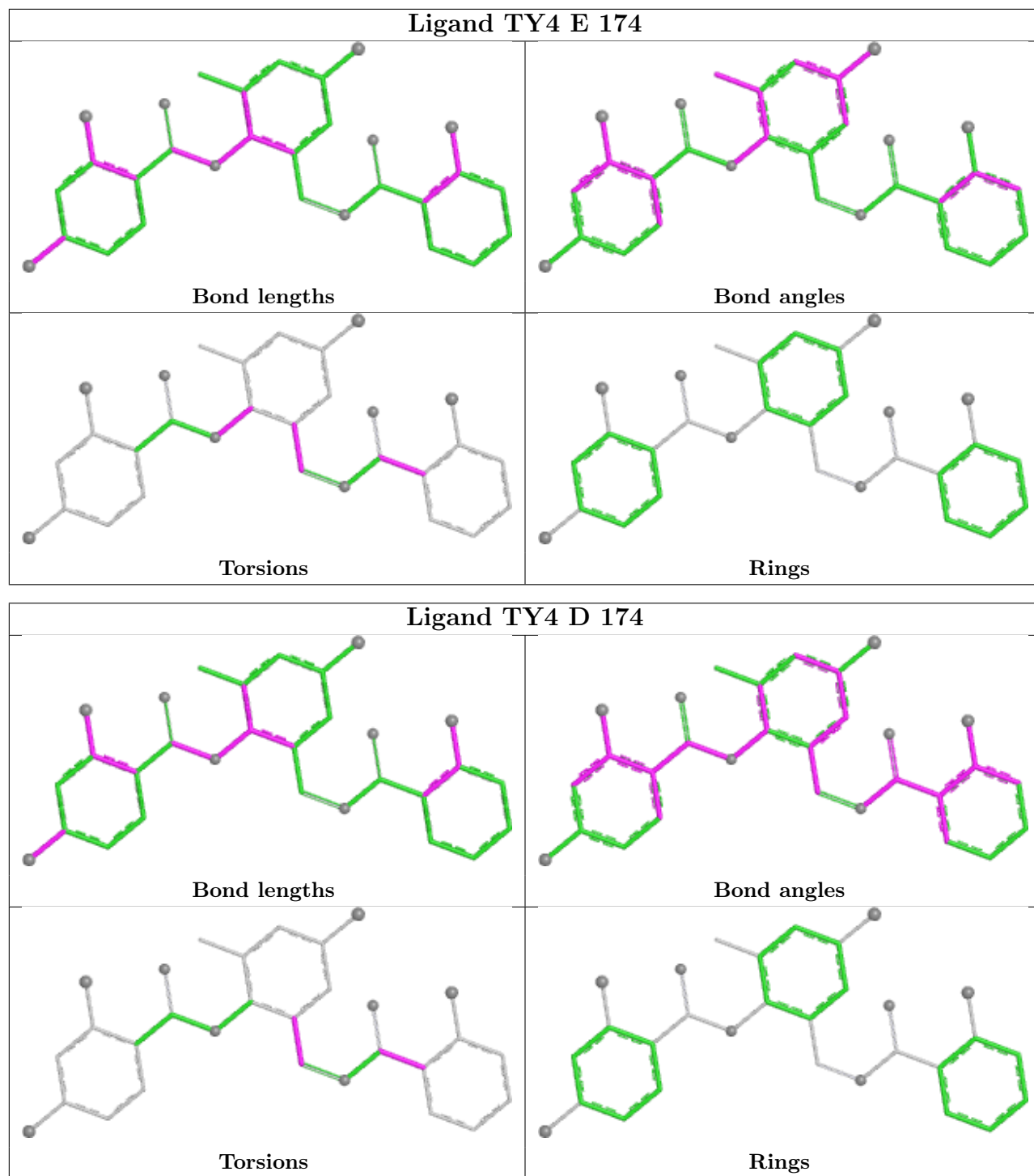


Ligand TY4 C 174



Ligand TY4 B 174





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	161/173 (93%)	0.42	4 (2%) 58 60	20, 28, 39, 44	0
1	B	161/173 (93%)	0.20	0 100 100	29, 35, 43, 50	0
1	C	163/173 (94%)	0.24	3 (1%) 67 69	30, 38, 48, 67	0
1	D	162/173 (93%)	0.85	13 (8%) 18 20	31, 39, 53, 67	0
1	E	161/173 (93%)	0.78	8 (4%) 34 35	33, 40, 46, 52	0
All	All	808/865 (93%)	0.50	28 (3%) 47 49	20, 38, 47, 67	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	ASP	3.7
1	E	123	GLY	3.6
1	D	153	MET	3.5
1	E	6	GLY	3.3
1	D	8	LEU	3.3
1	A	95	THR	3.3
1	E	120	GLY	2.9
1	D	67	ALA	2.8
1	E	93	TYR	2.7
1	A	11	GLU	2.7
1	D	12	ARG	2.6
1	C	50	ALA	2.6
1	D	121	ALA	2.6
1	D	64	TYR	2.5
1	D	7	PHE	2.5
1	D	166	ALA	2.5
1	E	166	ALA	2.5
1	E	100	GLU	2.4
1	A	48	GLU	2.4
1	D	15	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	157	TYR	2.2
1	E	121	ALA	2.2
1	C	8	LEU	2.1
1	D	60	TRP	2.1
1	A	138	ALA	2.1
1	E	10	LEU	2.1
1	C	68	GLY	2.0
1	D	5	ASP	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](#)

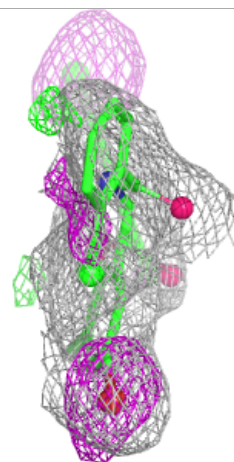
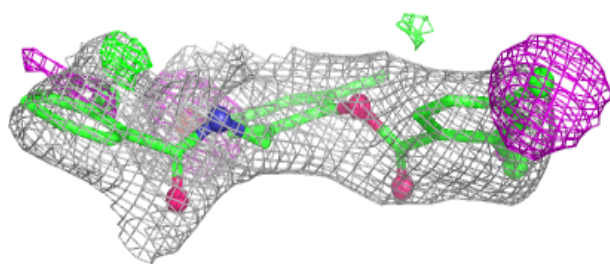
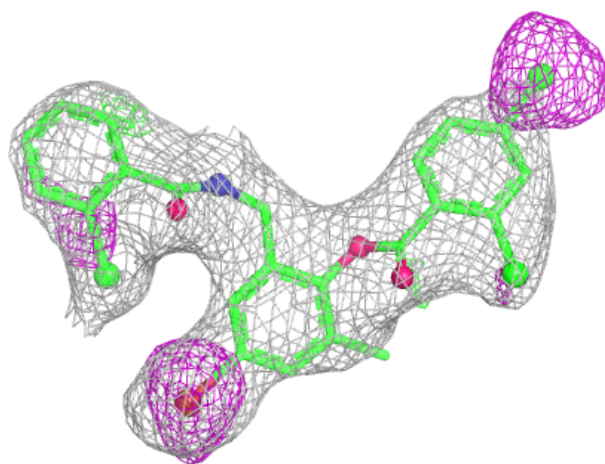
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	TY4	C	174	30/30	0.81	0.13	60,67,75,79	0
2	TY4	E	174	30/30	0.82	0.13	63,71,78,84	0
2	TY4	D	174	30/30	0.84	0.12	60,64,75,79	0
2	TY4	A	174	30/30	0.87	0.12	37,46,60,68	0
2	TY4	B	174	30/30	0.88	0.12	47,57,66,75	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.

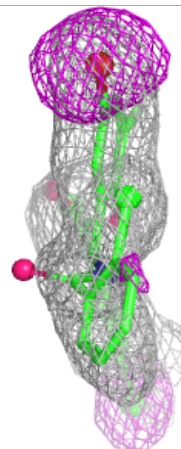
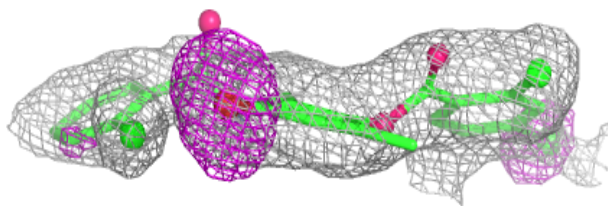
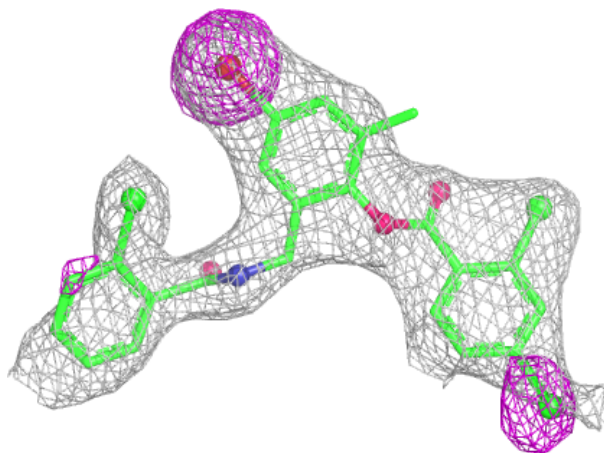
Electron density around TY4 C 174:

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



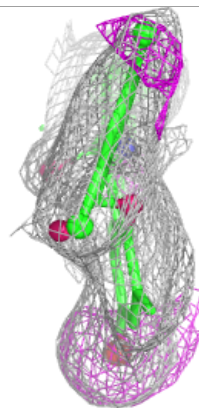
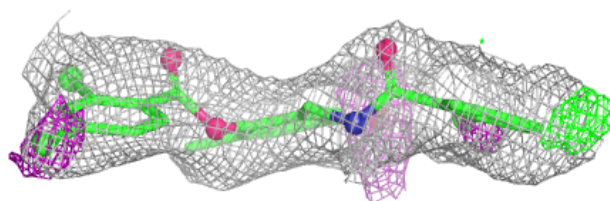
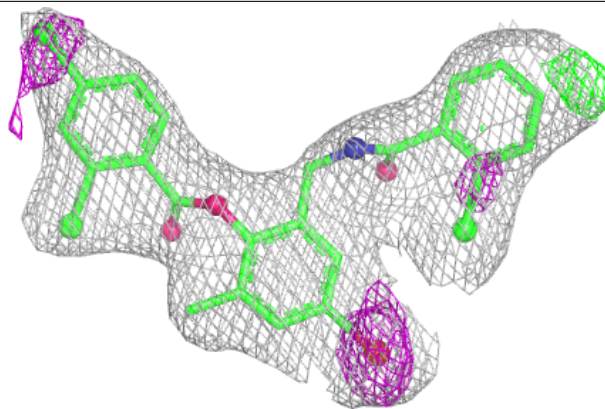
Electron density around TY4 E 174:

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



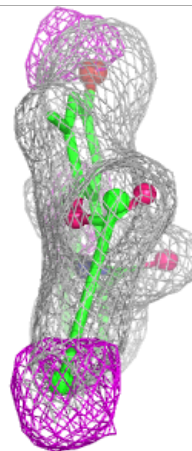
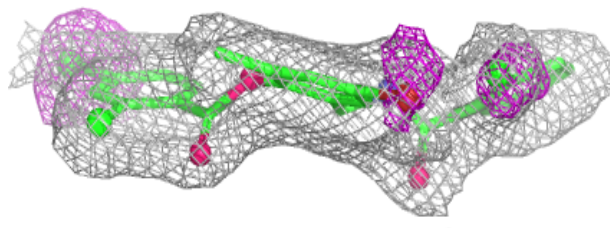
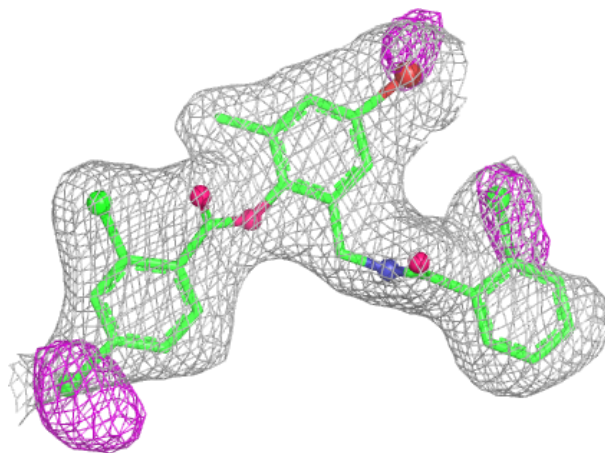
Electron density around TY4 D 174:

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



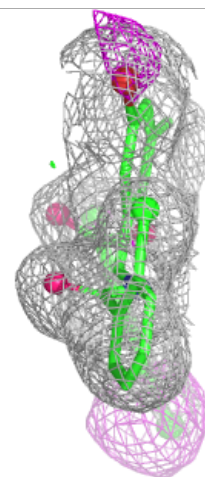
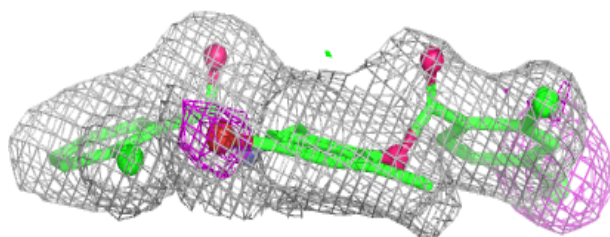
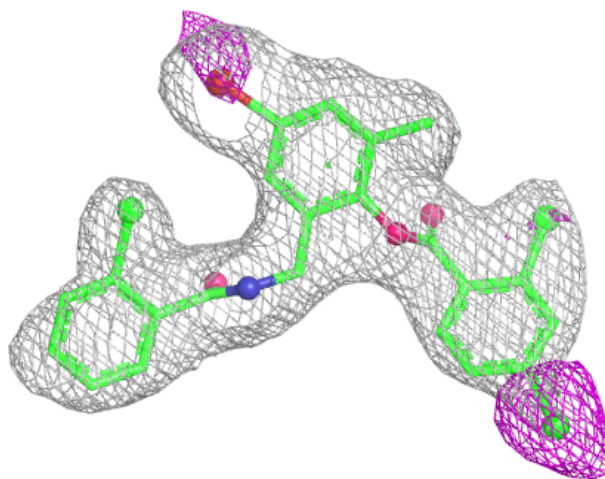
Electron density around TY4 A 174:

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



Electron density around TY4 B 174:

$2mF_o-DF_c$ (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.