



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:57 PM UTC

PDB ID : 5JHD / pdb_00005jhd
Title : Crystal structure of LS10-TCR/M1-HLA-A*02 complex
Authors : Stern, L.J.; Selin, L.K.; Song, I.
Deposited on : 2016-04-20
Resolution : 2.46 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

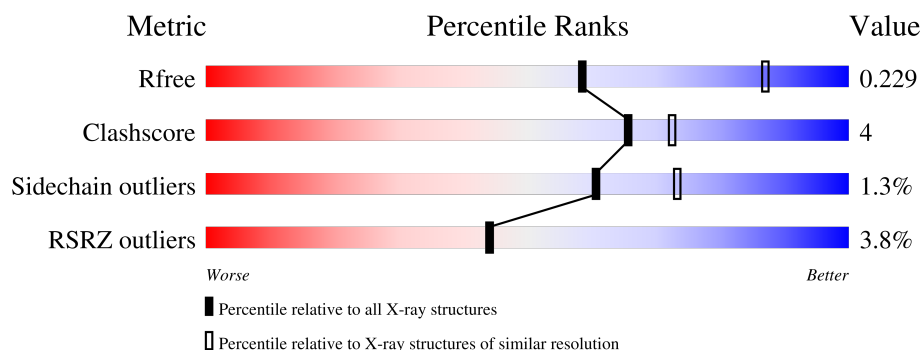
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	276	3% 92% 8%
1	F	276	4% 91% 9%
2	B	100	2% 96% .
2	G	100	% 94% 6%
3	C	9	89% 11%
3	H	9	89% 11%

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Mol	Chain	Length	Quality of chain
4	D	213	3% 88% 6% 6%
4	I	213	8% 85% 8% 5%
5	E	242	2% 89% 10%
5	J	242	5% 88% 10%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 26038 atoms, of which 12546 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	276	Total	C	H	N	O	S	0	2	0
			4378	1412	2115	414	428	9			
1	F	276	Total	C	H	N	O	S	0	1	0
			4339	1403	2091	409	427	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	ALA	-	expression tag	UNP P01892
F	276	ALA	-	expression tag	UNP P01892

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	100	Total	C	H	N	O	S	0	0	0
			1625	530	792	140	159	4			
2	G	100	Total	C	H	N	O	S	0	0	0
			1625	530	792	140	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Influenza M1(58-66) peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O		0	0	0
			144	49	75	9	11				
3	H	9	Total	C	H	N	O		0	0	0
			144	49	75	9	11				

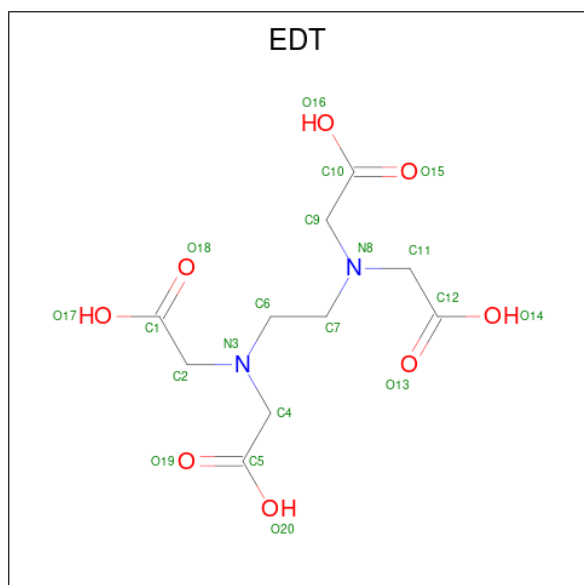
- Molecule 4 is a protein called TCRalpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	201	Total	C	H	N	O	S	0	0	0
			3078	995	1494	259	320	10			
4	I	203	Total	C	H	N	O	S	0	0	0
			3099	1003	1501	262	323	10			

- Molecule 5 is a protein called TCRbeta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	239	Total	C	H	N	O	S	0	0	0
			3691	1202	1793	327	363	6			
5	J	239	Total	C	H	N	O	S	0	0	0
			3692	1202	1794	327	363	6			

- Molecule 6 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: C₁₀H₁₆N₂O₈).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total	C	H	N	O		0	0
			32	10	12	2	8			
6	J	1	Total	C	H	N	O		0	0
			32	10	12	2	8			

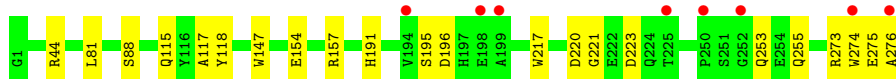
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	34	Total 34	O 34	0	0
7	B	13	Total 13	O 13	0	0
7	C	3	Total 3	O 3	0	0
7	D	17	Total 17	O 17	0	0
7	E	12	Total 12	O 12	0	0
7	F	40	Total 40	O 40	0	0
7	G	13	Total 13	O 13	0	0
7	I	13	Total 13	O 13	0	0
7	J	14	Total 14	O 14	0	0

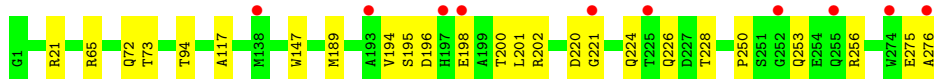
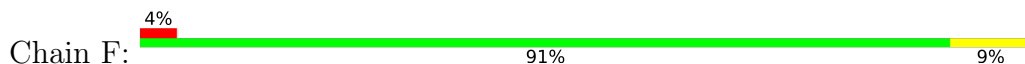
3 Residue-property plots [i](#)

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.

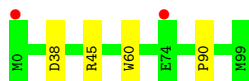
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



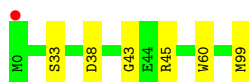
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: Influenza M1(58-66) peptide



- Molecule 3: Influenza M1(58-66) peptide

Chain H:  89% 11%



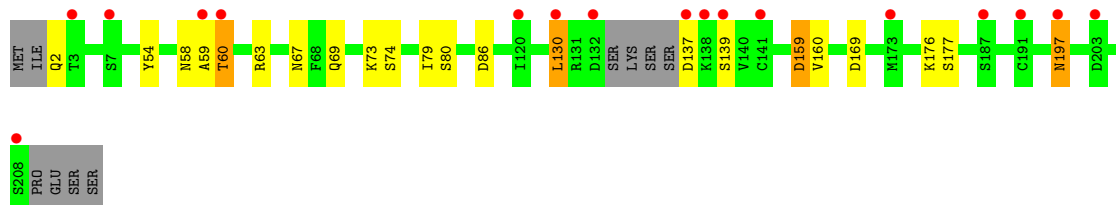
- Molecule 4: TCRalpha chain

Chain D:  3% 88% 6% 6%



- Molecule 4: TCRalpha chain

Chain I:  8% 85% 8% 5%



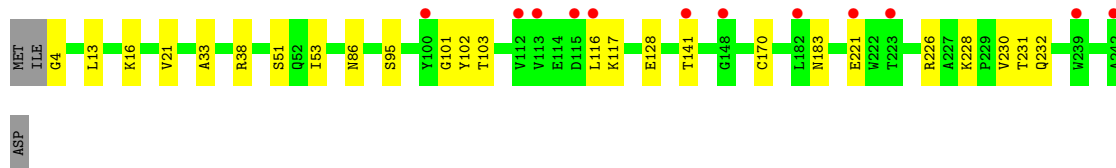
- Molecule 5: TCRbeta chain

Chain E:  2% 89% 10% 0%



- Molecule 5: TCRbeta chain

Chain J:  5% 88% 10% 0%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.71Å 101.84Å 113.55Å 99.38° 92.60° 103.45°	Depositor
Resolution (Å)	29.05 – 2.46 29.05 – 2.46	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.05-2.46) 88.6 (29.05-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.45Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.223 (Not available) , 0.229	Depositor DCC
R_{free} test set	3546 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.056 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26038	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.16	0/2333	0.34	0/3165
1	F	0.17	0/2318	0.34	0/3147
2	B	0.16	0/856	0.32	0/1158
2	G	0.16	0/856	0.31	0/1158
3	C	0.18	0/70	0.40	0/92
3	H	0.20	0/70	0.37	0/92
4	D	0.16	0/1619	0.37	0/2196
4	I	0.15	0/1633	0.37	0/2215
5	E	0.21	1/1950 (0.1%)	0.33	0/2656
5	J	0.20	1/1950 (0.1%)	0.33	0/2656
All	All	0.17	2/13655 (0.0%)	0.34	0/18535

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	228	LYS	C-N	6.53	1.49	1.33
5	J	228	LYS	C-N	6.00	1.47	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	2115	2109	20	0
1	F	2248	2091	2085	20	0
2	B	833	792	792	2	1
2	G	833	792	792	6	0
3	C	69	75	75	1	0
3	H	69	75	75	1	0
4	D	1584	1494	1492	9	0
4	I	1598	1501	1502	19	0
5	E	1898	1793	1793	13	0
5	J	1898	1794	1794	13	0
6	E	20	12	12	0	0
6	J	20	12	12	1	1
7	A	34	0	0	5	0
7	B	13	0	0	0	0
7	C	3	0	0	0	0
7	D	17	0	0	2	0
7	E	12	0	0	4	0
7	F	40	0	0	7	0
7	G	13	0	0	3	0
7	I	13	0	0	8	0
7	J	14	0	0	2	0
All	All	13492	12546	12533	98	1

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 4.

All (98) 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)
4:D:6:GLN:O	7:D:301:HOH:O	1.82	0.96
4:I:2:GLN:OE1	7:I:301:HOH:O	1.85	0.94
5:J:4:GLY:N	7:J:401:HOH:O	2.02	0.91
5:E:147:THR:O	7:E:401:HOH:O	1.95	0.83
4:D:74:SER:OG	7:D:302:HOH:O	1.98	0.82
4:I:160:VAL:N	7:I:305:HOH:O	2.13	0.81
4:I:137:ASP:O	7:I:302:HOH:O	1.99	0.81
1:F:21:ARG:NE	7:F:301:HOH:O	2.06	0.77
4:I:74:SER:OG	7:I:303:HOH:O	2.02	0.76
5:E:123:GLU:N	7:E:401:HOH:O	2.19	0.75
4:I:139:SER:O	7:I:304:HOH:O	2.06	0.74
1:F:224:GLN:O	7:F:302:HOH:O	2.06	0.72
5:E:123:GLU:O	7:E:401:HOH:O	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:HG3	7:A:320:HOH:O	1.93	0.69
2:G:38:ASP:OD1	7:G:101:HOH:O	2.10	0.68
1:A:115:GLN:NE2	7:A:304:HOH:O	2.29	0.65
2:G:43:GLY:N	7:G:103:HOH:O	2.22	0.64
5:E:221:GLU:N	5:E:221:GLU:OE2	2.31	0.63
4:I:59:ALA:HB1	4:I:60:THR:HA	1.80	0.62
5:J:38:ARG:NH2	5:J:86:ASN:O	2.32	0.62
5:J:221:GLU:OE1	5:J:221:GLU:N	2.33	0.61
1:A:253:GLN:N	1:A:253:GLN:OE1	2.33	0.61
1:F:226:GLN:O	7:F:302:HOH:O	2.16	0.60
1:F:253:GLN:N	1:F:253:GLN:OE1	2.34	0.60
1:F:220:ASP:N	1:F:221:GLY:HA3	2.18	0.58
1:A:220:ASP:N	1:A:221:GLY:HA3	2.20	0.57
4:D:59:ALA:HB1	4:D:60:THR:HA	1.86	0.57
4:I:79:ILE:HA	7:I:307:HOH:O	2.06	0.55
4:I:63:ARG:NH2	4:I:86:ASP:OD2	2.39	0.55
5:J:117:LYS:O	5:J:226:ARG:NH2	2.40	0.54
4:I:159:ASP:N	4:I:159:ASP:OD1	2.41	0.54
4:I:59:ALA:HB1	4:I:60:THR:HG23	1.88	0.54
1:F:65:ARG:NH2	7:F:307:HOH:O	2.41	0.53
4:I:197:ASN:O	4:I:197:ASN:ND2	2.37	0.53
1:F:72:GLN:HG3	7:F:303:HOH:O	2.09	0.52
2:G:38:ASP:OD1	2:G:45:ARG:NE	2.43	0.52
1:F:94:THR:OG1	7:F:304:HOH:O	2.19	0.51
2:G:33:SER:OG	7:G:102:HOH:O	2.13	0.50
1:F:195:SER:O	1:F:196:ASP:C	2.53	0.50
4:I:130:LEU:HD12	4:I:130:LEU:N	2.27	0.49
4:I:58:ASN:O	4:I:59:ALA:HB3	2.12	0.49
4:D:58:ASN:O	4:D:59:ALA:HB3	2.12	0.49
1:F:202:ARG:NE	2:G:99:MET:O	2.42	0.47
4:I:69:GLN:O	4:I:73:LYS:N	2.48	0.46
1:A:191:HIS:HB2	1:A:274:TRP:CH2	2.50	0.46
1:A:274:TRP:CD2	1:A:275:GLU:HA	2.50	0.46
1:F:228:THR:HB	7:F:302:HOH:O	2.15	0.46
1:A:157[A]:ARG:NH1	7:A:309:HOH:O	2.48	0.46
6:J:301:EDT:H041	7:J:409:HOH:O	2.16	0.45
1:A:275:GLU:HG3	1:A:276:ALA:N	2.32	0.45
4:I:67:ASN:O	7:I:303:HOH:O	2.21	0.45
1:F:117:ALA:HB2	2:G:60:TRP:CE2	2.52	0.45
4:I:169:ASP:OD2	4:I:176:LYS:NZ	2.50	0.44
1:A:255:GLN:O	1:A:273:ARG:NH2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:198:GLU:HA	1:F:250:PRO:HA	2.00	0.44
5:E:118:ASN:ND2	5:E:184:ASP:OD2	2.50	0.44
1:F:147:TRP:CZ2	3:H:9:LEU:HD23	2.53	0.43
5:E:116:LEU:HD11	5:E:216:LEU:HD21	1.99	0.43
1:A:44:ARG:NH1	7:A:310:HOH:O	2.51	0.43
1:A:274:TRP:CE3	1:A:275:GLU:HA	2.53	0.43
1:A:196:ASP:OD2	1:A:196:ASP:N	2.50	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.43
5:E:33:ALA:HA	5:E:51:SER:O	2.18	0.43
4:D:63:ARG:NH2	4:D:86:ASP:OD2	2.52	0.43
5:E:116:LEU:O	5:E:116:LEU:HD13	2.19	0.43
5:J:230:VAL:O	5:J:232:GLN:HG2	2.19	0.43
1:F:189:MET:HE2	1:F:201:LEU:HD22	2.01	0.43
1:F:194:VAL:CG2	1:F:200:THR:HG23	2.49	0.43
1:F:275:GLU:HG3	1:F:276:ALA:N	2.34	0.43
1:A:275:GLU:O	1:A:276:ALA:HB2	2.19	0.43
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.54	0.42
5:J:33:ALA:HA	5:J:51:SER:O	2.19	0.42
4:I:59:ALA:HB1	4:I:60:THR:CA	2.48	0.42
4:D:25:TYR:OH	4:D:32:TYR:OH	2.11	0.42
4:D:60:THR:HG21	4:D:64:PHE:O	2.19	0.42
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.54	0.41
4:D:59:ALA:HB1	4:D:60:THR:CA	2.50	0.41
5:E:54:VAL:HG23	5:E:70:ARG:O	2.19	0.41
5:J:13:LEU:HD21	5:J:21:VAL:HG11	2.02	0.41
4:D:120:ILE:CD1	4:D:147:ASP:HA	2.50	0.41
5:J:230:VAL:HG12	5:J:231:THR:N	2.35	0.41
5:E:38:ARG:NH2	5:E:40:ASP:OD2	2.53	0.41
5:E:172:ASP:OD2	7:E:402:HOH:O	2.22	0.41
5:J:101:GLY:O	5:J:103:THR:HG23	2.20	0.41
2:B:38:ASP:OD1	2:B:45:ARG:NE	2.53	0.41
4:I:130:LEU:HB3	5:J:128:GLU:O	2.20	0.41
1:A:195:SER:OG	1:A:196:ASP:OD2	2.37	0.41
5:J:16:LYS:HE3	5:J:116:LEU:HD11	2.02	0.41
5:J:183:ASN:OD1	5:J:183:ASN:N	2.53	0.41
1:A:274:TRP:HA	1:A:275:GLU:HA	1.86	0.41
1:F:73:THR:HA	5:J:53:ILE:HD13	2.03	0.41
1:A:217:TRP:O	1:A:223:ASP:HA	2.21	0.41
1:A:88:SER:O	7:A:301:HOH:O	2.22	0.40
5:E:230:VAL:HG22	5:E:231:THR:N	2.37	0.40
1:F:220:ASP:OD2	1:F:256:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:38:ARG:HB2	5:E:48:ILE:HD11	2.03	0.40
1:F:194:VAL:HG23	1:F:200:THR:HG23	2.03	0.40
4:I:80:SER:N	7:I:307:HOH:O	2.33	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:PRO:O	6:J:301:EDT:O13[1_655]	1.27	0.93

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/231 (100%)	232 (100%)	0	100	100
1	F	230/231 (100%)	230 (100%)	0	100	100
2	B	94/95 (99%)	94 (100%)	0	100	100
2	G	94/95 (99%)	94 (100%)	0	100	100
3	C	7/7 (100%)	7 (100%)	0	100	100
3	H	7/7 (100%)	7 (100%)	0	100	100
4	D	179/191 (94%)	176 (98%)	3 (2%)	53	67
4	I	180/191 (94%)	174 (97%)	6 (3%)	33	48
5	E	204/210 (97%)	198 (97%)	6 (3%)	37	52
5	J	204/210 (97%)	200 (98%)	4 (2%)	48	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1431/1468 (98%)	1412 (99%)	19 (1%)	61	73

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	60	THR
4	D	107	THR
4	D	159	ASP
5	E	13	LEU
5	E	95	SER
5	E	102	TYR
5	E	170	CYS
5	E	182	LEU
5	E	224	GLN
4	I	54	TYR
4	I	60	THR
4	I	130	LEU
4	I	159	ASP
4	I	177	SER
4	I	197	ASN
5	J	95	SER
5	J	102	TYR
5	J	141	THR
5	J	170	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	255	GLN
2	B	13	HIS
5	E	206	HIS
1	F	54	GLN
1	F	224	GLN
2	G	13	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	EDT	E	301	-	19,19,19	1.10	0	24,24,24	1.39	3 (12%)
6	EDT	J	301	-	19,19,19	1.00	0	24,24,24	1.29	1 (4%)

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
6	EDT	E	301	-	-	10/21/21/21	-
6	EDT	J	301	-	-	2/21/21/21	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	301	EDT	C11-N8-C7	2.86	118.80	111.91
6	J	301	EDT	C11-N8-C7	-2.19	106.64	111.91
6	E	301	EDT	C6-C7-N8	-2.14	107.89	112.98
6	E	301	EDT	C10-C9-N8	-2.05	107.27	113.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

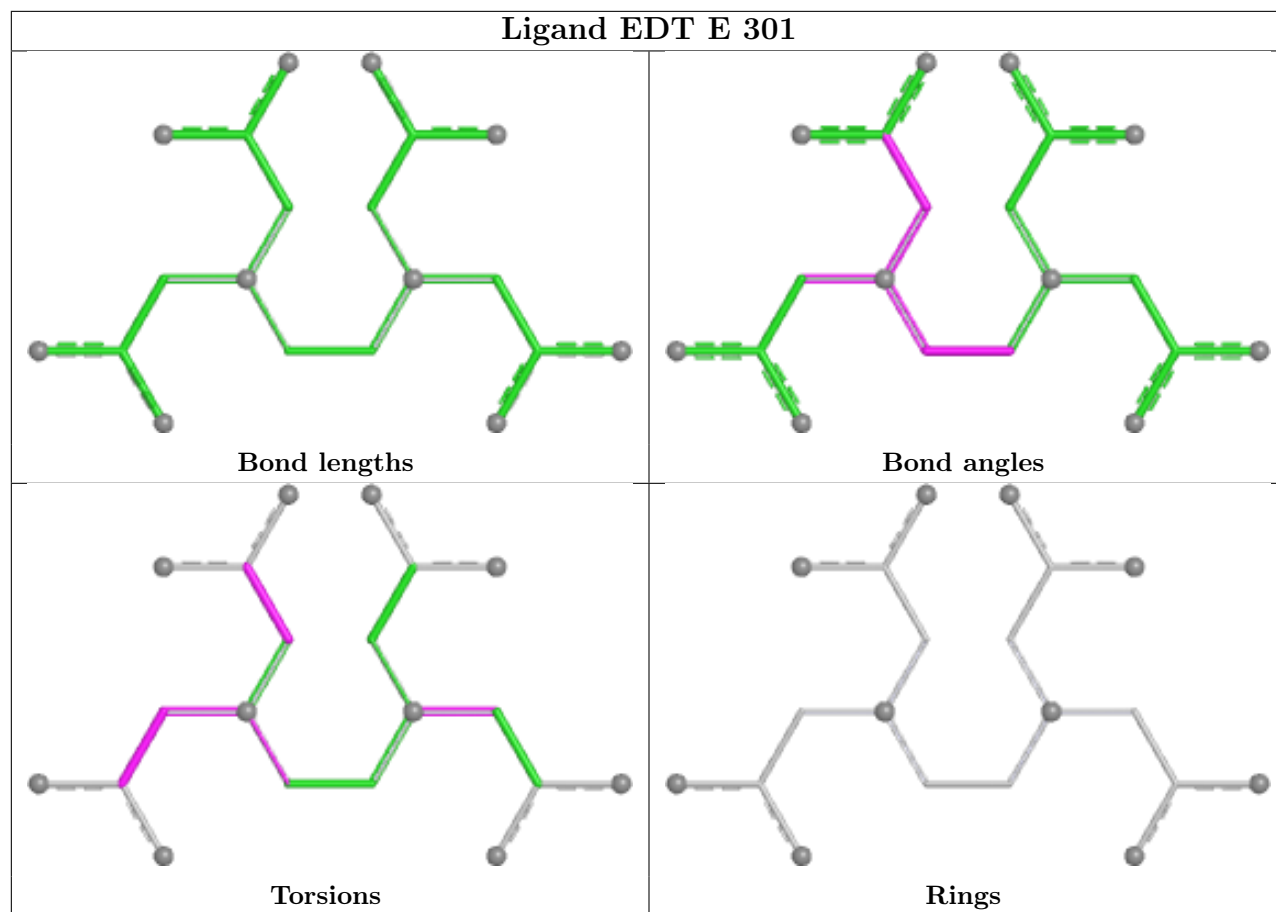
Mol	Chain	Res	Type	Atoms
6	E	301	EDT	C12-C11-N8-C7
6	E	301	EDT	O16-C10-C9-N8
6	E	301	EDT	O15-C10-C9-N8
6	E	301	EDT	N8-C11-C12-O14
6	E	301	EDT	N8-C11-C12-O13
6	E	301	EDT	C6-C7-N8-C11
6	E	301	EDT	C5-C4-N3-C2
6	E	301	EDT	C6-C7-N8-C9
6	E	301	EDT	C5-C4-N3-C6
6	E	301	EDT	C12-C11-N8-C9
6	J	301	EDT	C10-C9-N8-C11
6	J	301	EDT	C5-C4-N3-C6

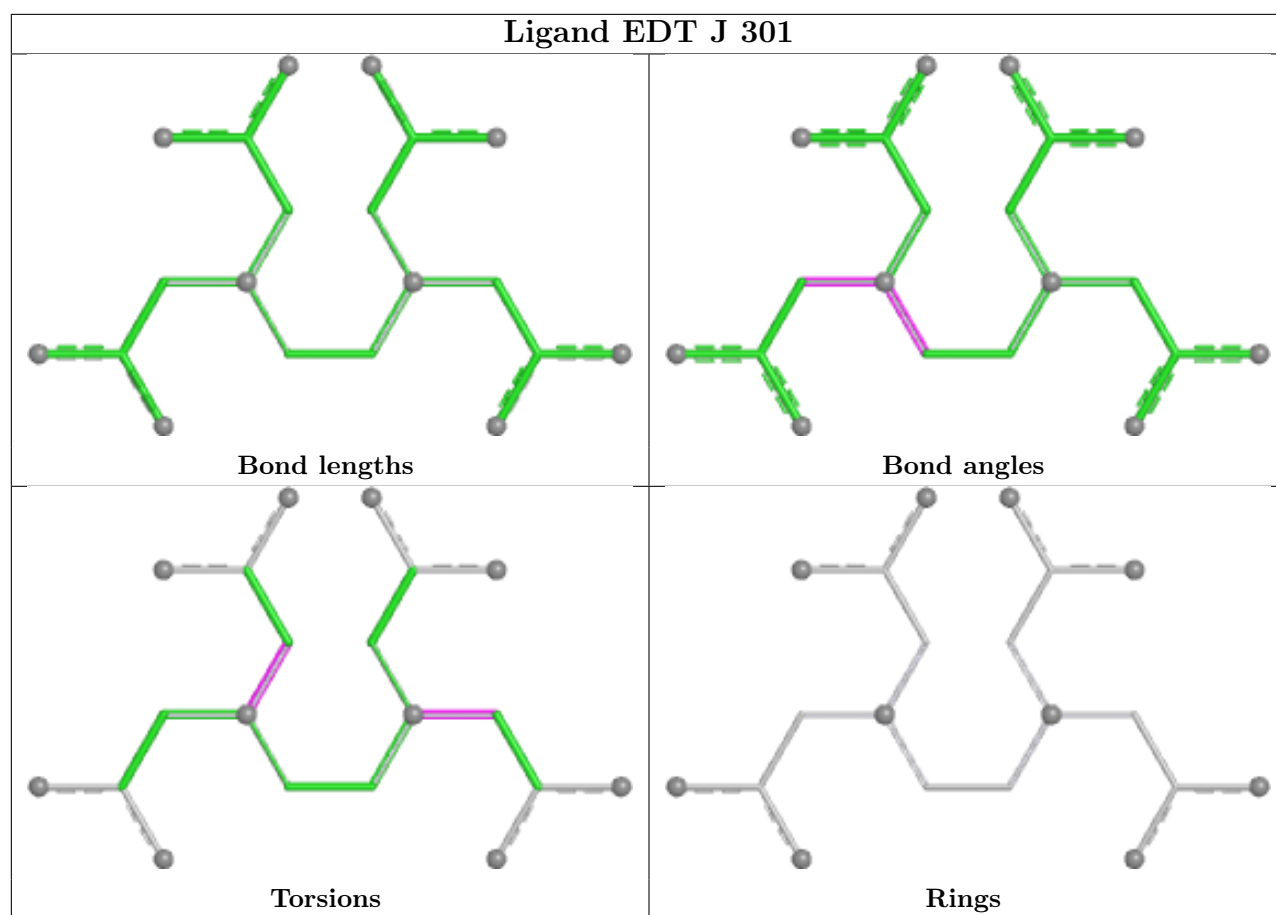
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	301	EDT	1	1

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.





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	276/276 (100%)	0.12	8 (2%) 53 55	28, 56, 142, 160	1 (0%)
1	F	276/276 (100%)	0.15	10 (3%) 46 46	29, 53, 150, 203	0
2	B	100/100 (100%)	-0.24	2 (2%) 65 66	27, 41, 83, 105	0
2	G	100/100 (100%)	-0.21	1 (1%) 79 80	27, 45, 87, 104	0
3	C	9/9 (100%)	-0.29	0 100 100	37, 43, 49, 49	0
3	H	9/9 (100%)	-0.15	0 100 100	38, 41, 44, 51	0
4	D	201/213 (94%)	0.55	7 (3%) 47 47	48, 77, 121, 155	0
4	I	203/213 (95%)	0.76	17 (8%) 17 15	38, 91, 132, 148	0
5	E	239/242 (98%)	0.49	6 (2%) 58 61	40, 79, 132, 157	0
5	J	239/242 (98%)	0.55	12 (5%) 34 32	32, 81, 139, 178	0
All	All	1652/1680 (98%)	0.32	63 (3%) 44 44	27, 68, 134, 203	1 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	J	242	ALA	5.6
1	A	276	ALA	4.4
4	I	137	ASP	4.2
5	J	239	TRP	3.8
4	I	208	SER	3.7
1	F	276	ALA	3.7
1	F	274	TRP	3.6
2	B	0	MET	3.6
4	I	60	THR	3.4
1	F	225	THR	3.4
4	I	139	SER	3.2
5	E	215	GLY	3.2
5	J	115	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
4	I	203	ASP	3.0
4	D	54	TYR	2.9
5	E	14	PHE	2.9
4	D	120	ILE	2.9
4	D	185	ASN	2.8
5	J	182	LEU	2.8
1	F	138	MET	2.8
1	F	255	GLN	2.7
4	I	138	LYS	2.7
4	D	59	ALA	2.6
5	J	116	LEU	2.6
4	I	59	ALA	2.6
1	F	193	ALA	2.5
4	I	191	CYS	2.5
1	F	197	HIS	2.5
5	E	115	ASP	2.5
5	J	113	VAL	2.5
2	G	0	MET	2.5
4	I	7	SER	2.5
1	F	198	GLU	2.4
1	F	221	GLY	2.4
1	F	252	GLY	2.4
5	E	242	ALA	2.4
4	D	101	THR	2.3
1	A	252	GLY	2.3
5	J	148	GLY	2.3
4	I	130	LEU	2.3
4	I	141	CYS	2.3
5	E	83	ALA	2.3
4	I	120	ILE	2.3
4	I	3	THR	2.2
5	J	221	GLU	2.2
5	J	112	VAL	2.2
1	A	274	TRP	2.2
4	D	71	ALA	2.2
1	A	198	GLU	2.2
2	B	74	GLU	2.2
5	E	117	LYS	2.2
4	I	132	ASP	2.1
4	D	187	SER	2.1
4	I	187	SER	2.1
5	J	141	THR	2.1

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Mol	Chain	Res	Type	RSRZ
5	J	223	THR	2.1
1	A	250	PRO	2.1
1	A	194	VAL	2.1
1	A	199	ALA	2.0
4	I	197	ASN	2.0
5	J	100	TYR	2.0
4	I	173	MET	2.0
1	A	225	THR	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

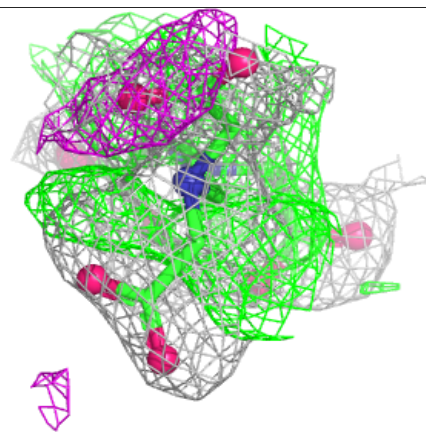
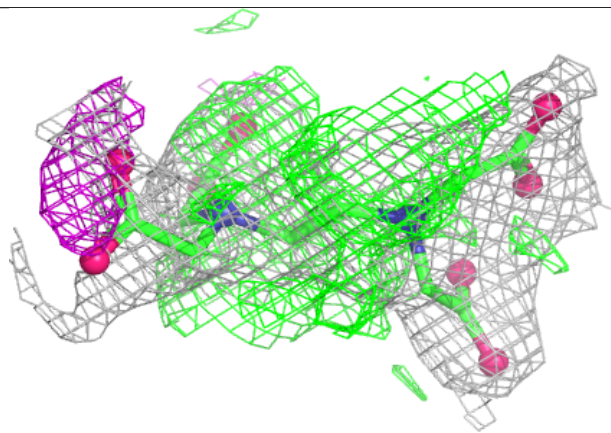
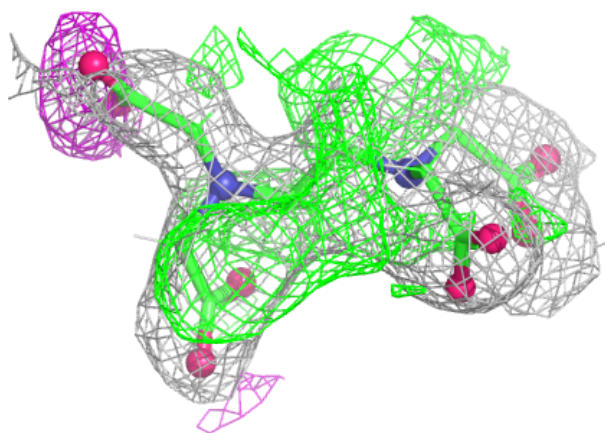
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDT	J	301	20/20	0.64	0.23	29,37,44,47	32
6	EDT	E	301	20/20	0.66	0.21	26,36,45,45	32

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.

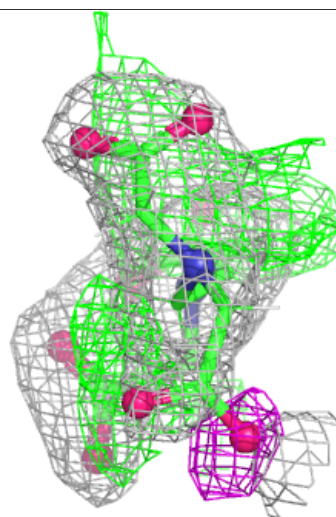
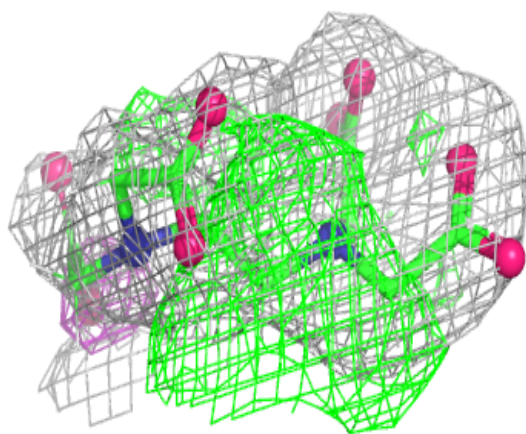
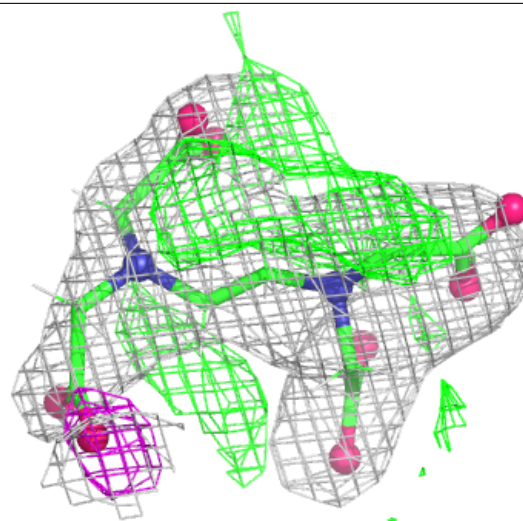
Electron density around EDT J 301:

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



Electron density around EDT E 301:

$2mF_o-DF_c$ (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.