Preliminary Full wwPDB X-ray Structure Validation Report (i)

Apr 16, 2021 – 12:30 AM EDT

Deposition ID : D_1000253296

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

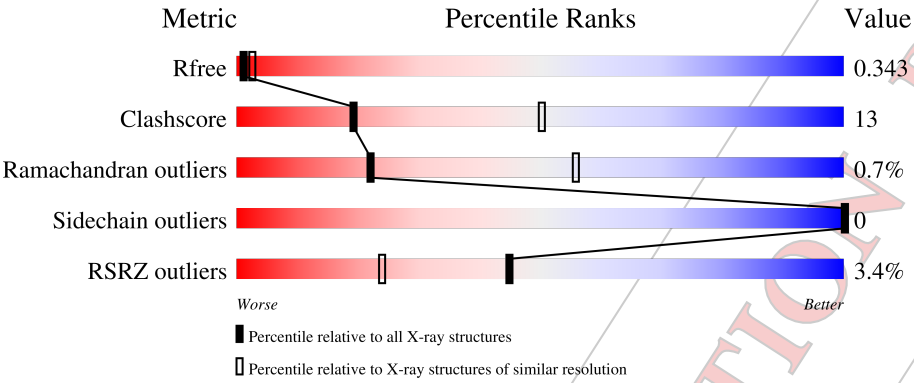
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.18
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.18

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 3.11 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 <=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	259	72% 26%
1	B	259	5% 75% 23%
1	C	259	4% 78% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5324 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	1762	1112	290	345	15	0	1	0
1	B	253	Total	C	N	O	S	0	0	0
			1711	1076	289	334	12			
1	C	248	Total	C	N	O	S	0	0	0
			1700	1086	281	320	13			

- Molecule 2 is a ligand with the chemical component id LIG but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LIG. Consequently no firm identification of ligand chemistry can be made. Once the structure is annotated then an identification and diagram will be given here.

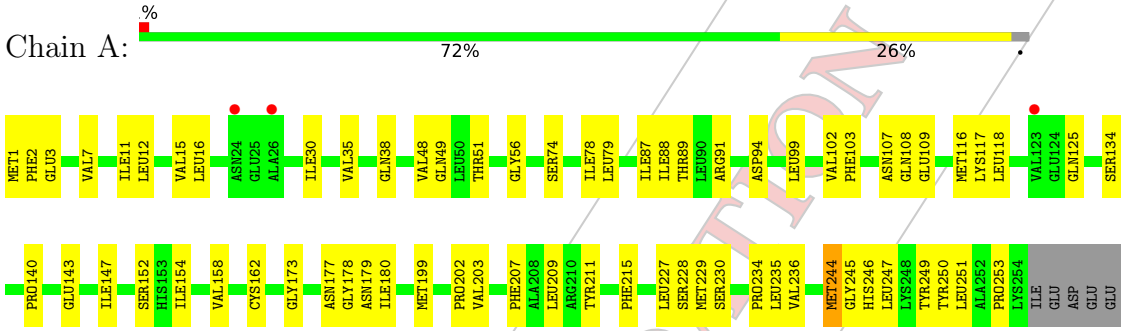
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	E	1	74	49	10	12	3	0	0
2	D	1	Total	C	N	O	S	0	0
			77	51	10	13	3		

3 Residue-property plots

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.

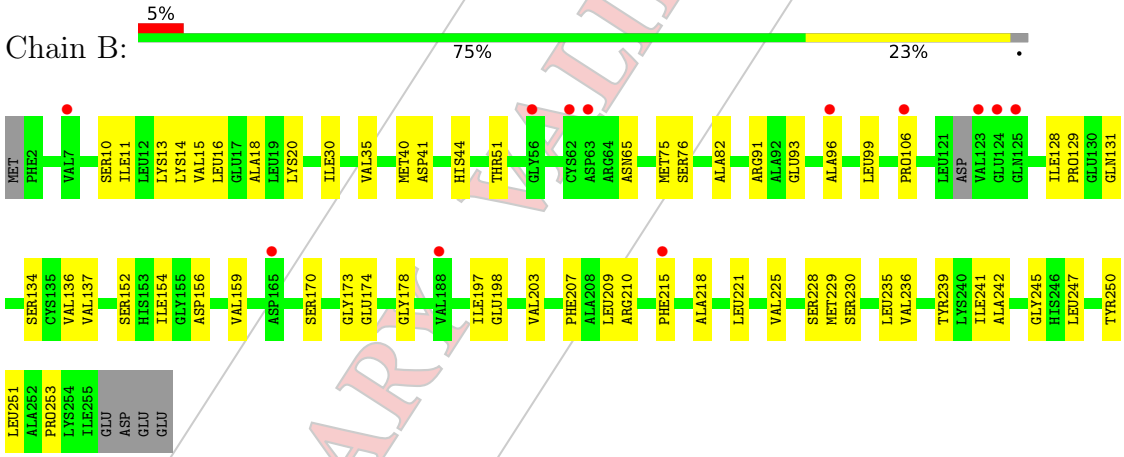
• Molecule 1: Proliferating cell nuclear antigen

Chain A:



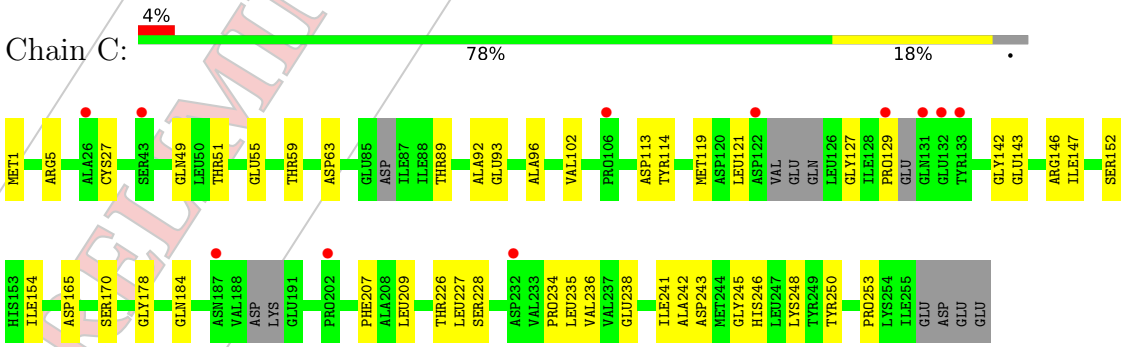
• Molecule 1: Proliferating cell nuclear antigen

Chain B:



• Molecule 1: Proliferating cell nuclear antigen

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	83.36Å 83.36Å 181.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.37 – 3.11 38.37 – 3.11	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.37-3.11) 94.2 (38.37-3.11)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.272 , 0.309 0.288 , 0.343	Depositor DCC
R_{free} test set	624 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.884	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtriage
Reported twinning fraction	0.120 for -h,-k,l	Depositor
Outliers	1 of 12930 reflections (0.008%)	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	5324	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 7.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: LIG

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	0.27	0/1791	0.54	0/2444
1	B	0.28	0/1735	0.58	0/2373
1	C	0.27	0/1722	0.53	0/2348
All	All	0.28	0/5248	0.55	0/7165

There are no bond length outliers.

There are no bond angle outliers.

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	1762	0	1568	53	0
1	B	1711	0	1494	46	0
1	C	1700	0	1529	32	0
2	D	77	0	0	3	0
2	E	74	0	0	1	0
All	All	5324	0	4591	128	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 13.

All (128) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:THR:O	1:B:245:GLY:HA3	1.73	0.89
1:B:16:LEU:HD21	1:B:75:MET:HG2	1.59	0.82
1:C:5:ARG:HB2	1:C:59:THR:HB	1.65	0.79
2:E:1:LIG:N38	2:E:1:LIG:O82	2.19	0.75
1:B:228:SER:HB2	1:B:236:VAL:HB	1.69	0.75
1:A:1:MET:N	1:A:94:ASP:OD1	2.20	0.74
1:B:207:PHE:HE1	1:B:253:PRO:HG3	1.57	0.69
1:B:137:VAL:HG22	1:B:197:ILE:HG12	1.76	0.67
1:A:229:MET:HB3	1:A:235:LEU:HD13	1.77	0.66
1:B:215:PHE:HE2	1:B:251:LEU:HD22	1.60	0.66
1:C:51:THR:O	1:C:245:GLY:HA3	1.96	0.64
1:B:13:LYS:HE2	1:B:82:ALA:HB3	1.79	0.63
1:C:238:GLU:HG3	1:C:248:LYS:HG3	1.79	0.63
1:B:136:VAL:HB	1:B:198:GLU:HB2	1.79	0.62
1:B:235:LEU:HD23	1:B:251:LEU:HD21	1.81	0.62
1:B:93:GLU:HB3	1:B:96:ALA:HB3	1.82	0.62
1:C:241:ILE:O	1:C:243:ASP:N	2.34	0.60
1:C:165:ASP:O	1:C:184:GLN:N	2.34	0.60
1:A:7:VAL:HG13	1:A:87:ILE:HG12	1.83	0.59
1:C:27:CYS:SG	1:C:121:LEU:HD22	2.43	0.59
1:A:16:LEU:HG	1:A:79:LEU:HD13	1.84	0.59
1:A:30:ILE:HD12	1:A:35:VAL:HG12	1.85	0.59
1:C:228:SER:HB2	1:C:236:VAL:HB	1.85	0.58
1:B:241:ILE:HD11	1:B:247:LEU:HD23	1.86	0.58
1:A:51:THR:O	1:A:245:GLY:HA3	2.03	0.57
1:C:1:MET:N	1:C:63:ASP:OD2	2.34	0.57
1:A:134:SER:N	1:A:230:SER:OG	2.28	0.57
1:A:179:ASN:N	1:C:113:ASP:O	2.37	0.57
1:A:88:ILE:HG12	1:A:103:PHE:HD1	1.70	0.57
1:A:215:PHE:CE2	1:A:251:LEU:HG	2.40	0.57
1:B:30:ILE:O	1:B:65:ASN:HA	2.06	0.56
1:C:227:LEU:HD12	1:C:235:LEU:HD11	1.88	0.56
1:B:159:VAL:HB	1:B:170:SER:HB3	1.88	0.55
1:B:154:ILE:O	1:B:173:GLY:HA3	2.06	0.54
1:A:89:THR:HB	1:A:102:VAL:HB	1.90	0.54
1:B:229:MET:HG3	1:B:235:LEU:HD13	1.89	0.54
1:A:56:GLY:HA3	1:A:244:MET:HG3	1.89	0.54
1:C:89:THR:HB	1:C:102:VAL:HB	1.90	0.54
1:A:215:PHE:HE2	1:A:251:LEU:HG	1.71	0.53
1:B:40:MET:SD	1:B:44:HIS:ND1	2.74	0.53
1:A:3:GLU:HG2	1:A:91:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HB	1:A:209:LEU:HD21	1.90	0.52
1:C:55:GLU:OE1	1:C:55:GLU:N	2.36	0.52
1:B:18:ALA:HB1	1:B:218:ALA:HB2	1.91	0.52
1:C:142:GLY:O	1:C:146:ARG:HG3	2.09	0.52
1:A:107:ASN:O	1:A:109:GLU:N	2.43	0.51
1:B:128:ILE:O	1:B:128:ILE:HG13	2.10	0.51
2:D:301:LIG:OA1	2:D:301:LIG:N18	2.44	0.51
1:B:207:PHE:CZ	1:B:235:LEU:HB2	2.44	0.51
1:A:88:ILE:HG12	1:A:103:PHE:CD1	2.45	0.50
1:B:174:GLU:HA	1:C:119:MET:HA	1.93	0.50
1:B:203:VAL:HG11	1:B:229:MET:HB3	1.94	0.50
1:C:207:PHE:HE1	1:C:253:PRO:HB3	1.76	0.50
1:B:218:ALA:HB1	1:B:221:LEU:HD12	1.93	0.50
1:A:228:SER:HB2	1:A:236:VAL:HB	1.93	0.49
1:A:117:LYS:HG2	1:A:118:LEU:O	2.12	0.49
1:B:129:PRO:O	1:B:131:GLN:HG3	2.13	0.49
1:A:99:LEU:HB2	1:A:118:LEU:HD21	1.94	0.49
1:C:236:VAL:HG22	1:C:250:TYR:CD1	2.48	0.49
1:A:236:VAL:HG22	1:A:250:TYR:CD1	2.48	0.48
1:B:152:SER:HA	1:B:209:LEU:HD13	1.95	0.48
1:B:16:LEU:O	1:B:20:LYS:N	2.44	0.48
1:A:154:ILE:HD13	1:A:178:GLY:HA3	1.95	0.48
1:B:11:ILE:O	1:B:15:VAL:HG23	2.13	0.48
1:A:177:ASN:OD1	1:A:178:GLY:N	2.46	0.48
1:B:30:ILE:HD12	1:B:35:VAL:HG22	1.96	0.48
1:B:156:ASP:HB2	1:B:210:ARG:NH1	2.29	0.48
1:A:154:ILE:HD11	1:C:114:TYR:CE2	2.48	0.48
2:D:301:LIG:OA0	2:D:301:LIG:O27	2.25	0.47
1:A:203:VAL:HG21	1:A:229:MET:HG2	1.96	0.47
1:C:207:PHE:CE2	1:C:235:LEU:HD22	2.48	0.47
1:A:38:GLN:HA	1:A:48:VAL:O	2.15	0.47
1:A:154:ILE:HD11	1:C:114:TYR:CD2	2.50	0.47
1:A:179:ASN:O	1:C:113:ASP:N	2.45	0.47
1:A:247:LEU:HD21	1:A:249:TYR:OH	2.15	0.47
1:A:2:PHE:O	1:A:3:GLU:HG3	2.15	0.46
1:A:7:VAL:HA	1:A:87:ILE:HG12	1.97	0.46
1:A:152:SER:HA	1:A:209:LEU:HD13	1.98	0.46
1:B:91:ARG:O	1:B:99:LEU:HD12	2.16	0.46
1:C:234:PRO:HA	1:C:253:PRO:HD3	1.98	0.46
1:A:235:LEU:O	1:A:250:TYR:HA	2.16	0.45
1:C:49:GLN:OE1	1:C:246:HIS:NE2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PRO:HB2	1:A:143:GLU:OE1	2.17	0.45
1:A:162:CYS:HB3	1:A:203:VAL:HG22	1.97	0.45
1:B:40:MET:HG2	1:B:41:ASP:H	1.82	0.45
1:A:207:PHE:CZ	1:A:235:LEU:HB2	2.52	0.45
1:B:134:SER:H	1:B:230:SER:HG	1.58	0.45
1:B:218:ALA:HB3	1:B:239:TYR:CE2	2.52	0.44
1:A:227:LEU:HD12	1:A:235:LEU:HD11	1.98	0.44
1:A:12:LEU:O	1:A:16:LEU:HD23	2.17	0.44
1:B:10:SER:O	1:B:14:LYS:HG3	2.17	0.44
1:A:234:PRO:HA	1:A:251:LEU:O	2.18	0.44
1:B:225:VAL:HG23	1:B:239:TYR:CE1	2.53	0.44
1:C:152:SER:HA	1:C:209:LEU:HD13	1.98	0.44
1:C:207:PHE:CE1	1:C:253:PRO:HB3	2.53	0.44
1:C:154:ILE:HD13	1:C:178:GLY:HA3	2.00	0.43
1:A:211:TYR:HB3	1:A:251:LEU:HD21	2.01	0.43
1:A:116:MET:HE2	1:A:116:MET:HB2	1.56	0.43
1:B:235:LEU:O	1:B:250:TYR:HA	2.19	0.43
1:B:218:ALA:HB3	1:B:239:TYR:HE2	1.84	0.43
1:B:11:ILE:HD12	1:B:11:ILE:H	1.84	0.43
1:B:215:PHE:CE2	1:B:251:LEU:HD22	2.47	0.43
1:B:225:VAL:HG23	1:B:239:TYR:HE1	1.83	0.43
1:B:236:VAL:HG22	1:B:250:TYR:CE1	2.53	0.43
1:C:170:SER:HA	1:C:178:GLY:O	2.19	0.42
1:A:74:SER:O	1:A:78:ILE:HG13	2.18	0.42
1:B:241:ILE:HD11	1:B:247:LEU:CD2	2.49	0.42
1:A:2:PHE:O	1:A:91:ARG:HA	2.19	0.42
1:A:38:GLN:OE1	1:A:125:GLN:HG2	2.19	0.42
1:A:49:GLN:HG3	1:A:246:HIS:HE1	1.85	0.42
1:C:143:GLU:O	1:C:147:ILE:HG12	2.19	0.42
1:A:227:LEU:HD12	1:A:235:LEU:HD21	2.01	0.42
1:C:1:MET:HG3	1:C:92:ALA:O	2.20	0.42
1:C:93:GLU:HB2	1:C:96:ALA:HB2	2.01	0.42
1:C:226:THR:OG1	1:C:238:GLU:HB3	2.20	0.42
1:A:199:MET:SD	1:A:202:PRO:HG3	2.59	0.42
1:A:178:GLY:HA2	1:C:114:TYR:HA	2.01	0.42
1:A:147:ILE:HG12	1:A:180:ILE:HG21	2.02	0.41
1:A:253:PRO:HD2	2:D:301:LIG:C86	2.51	0.41
1:B:93:GLU:HB3	1:B:96:ALA:CB	2.49	0.41
1:A:11:ILE:O	1:A:15:VAL:HG23	2.20	0.41
1:B:207:PHE:CE2	1:B:235:LEU:HB2	2.55	0.41
1:C:127:GLY:O	1:C:129:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:VAL:HG22	1:B:250:TYR:CD1	2.56	0.41
1:B:16:LEU:HD23	1:B:76:SER:HA	2.03	0.41
1:B:170:SER:HA	1:B:178:GLY:O	2.20	0.41
1:A:143:GLU:OE1	1:A:143:GLU:N	2.52	0.40
1:A:154:ILE:O	1:A:173:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	253/259 (98%)	238 (94%)	13 (5%)	2 (1%)	19	53
1	B	249/259 (96%)	230 (92%)	17 (7%)	2 (1%)	19	53
1	C	238/259 (92%)	227 (95%)	10 (4%)	1 (0%)	34	68
All	All	740/777 (95%)	695 (94%)	40 (5%)	5 (1%)	22	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	242	ALA
1	A	244	MET
1	B	106	PRO
1	B	242	ALA
1	A	108	GLN

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	161/227 (71%)	161 (100%)	0	100	100
1	B	151/227 (66%)	151 (100%)	0	100	100
1	C	149/227 (66%)	149 (100%)	0	100	100
All	All	461/681 (68%)	461 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	254/259 (98%)	-0.05	3 (1%) 79 63	37, 54, 84, 113	0
1	B	253/259 (97%)	0.06	12 (4%) 31 14	42, 56, 86, 116	0
1	C	248/259 (95%)	0.10	11 (4%) 34 17	47, 62, 92, 121	0
All	All	755/777 (97%)	0.04	26 (3%) 45 24	37, 57, 91, 121	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	ALA	4.3
1	C	132	GLU	3.5
1	B	96	ALA	3.5
1	C	131	GLN	3.2
1	B	188	VAL	3.1
1	A	123	VAL	3.0
1	B	62	CYS	3.0
1	B	125	GLN	2.9
1	A	26	ALA	2.8
1	C	43	SER	2.7
1	C	129	PRO	2.7
1	B	215	PHE	2.6
1	A	24	ASN	2.6
1	C	106	PRO	2.5
1	B	106	PRO	2.4
1	B	7	VAL	2.4
1	C	232	ASP	2.4
1	B	165	ASP	2.3
1	C	202	PRO	2.3
1	B	123	VAL	2.2
1	C	122	ASP	2.2
1	B	124	GLU	2.2
1	B	56	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	63	ASP	2.1
1	C	187	ASN	2.0
1	C	133	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

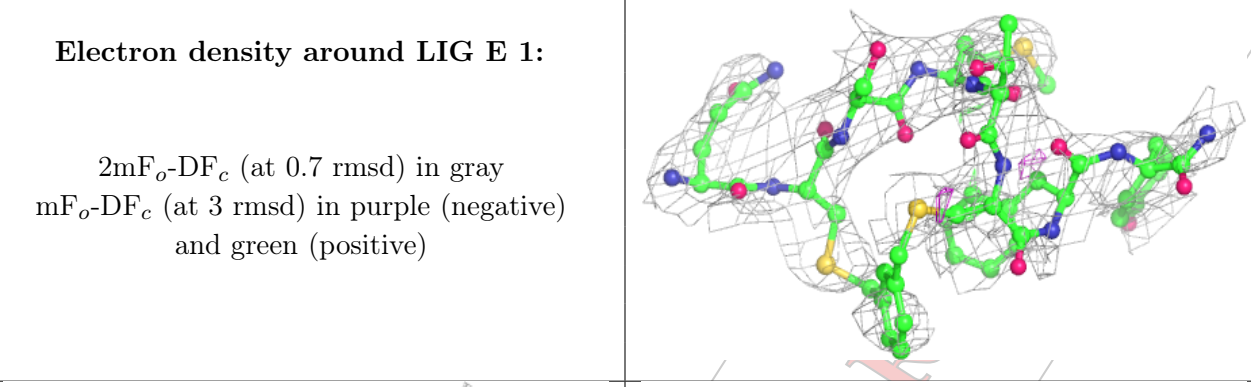
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

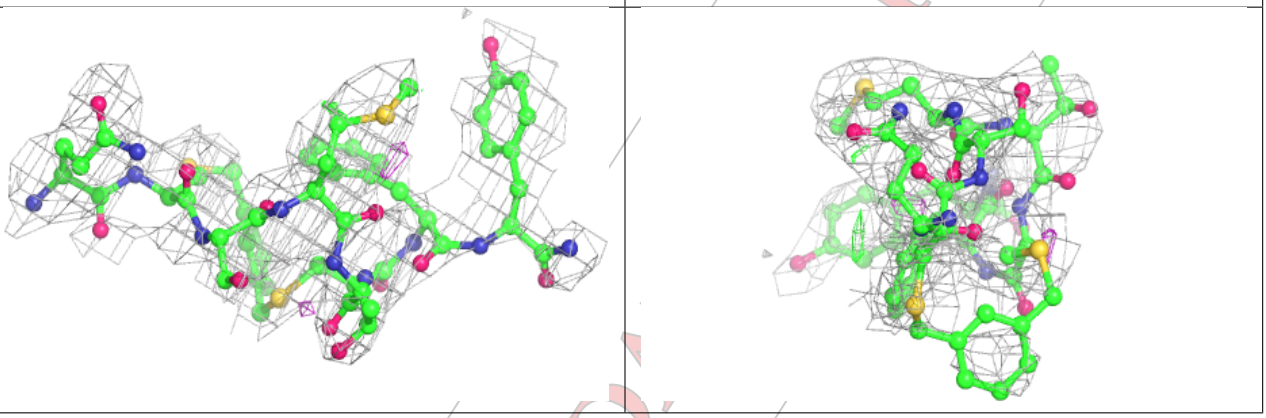
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIG	E	1	74/?	0.78	0.32	43,72,90,99	0
2	LIG	D	301	77/?	0.81	0.25	43,62,78,83	0

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 LIG E 1:

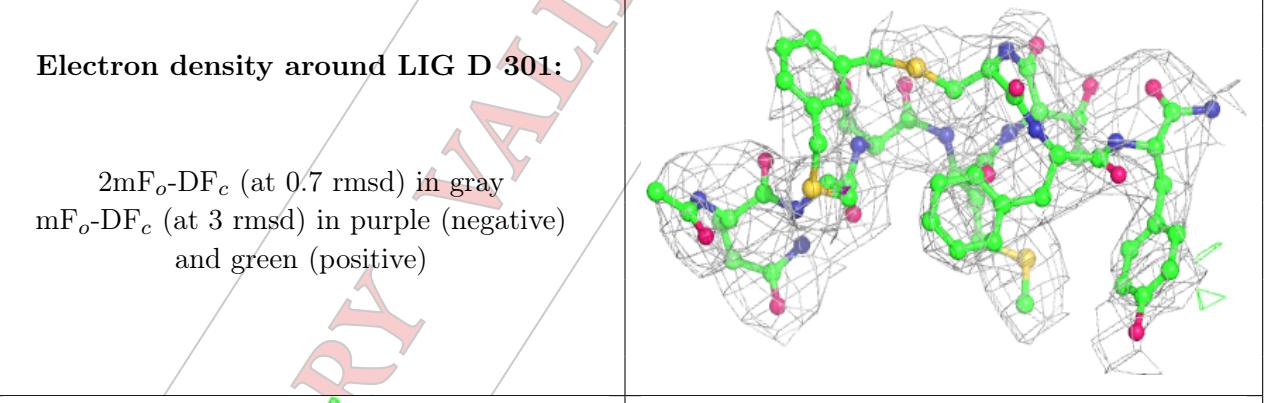
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

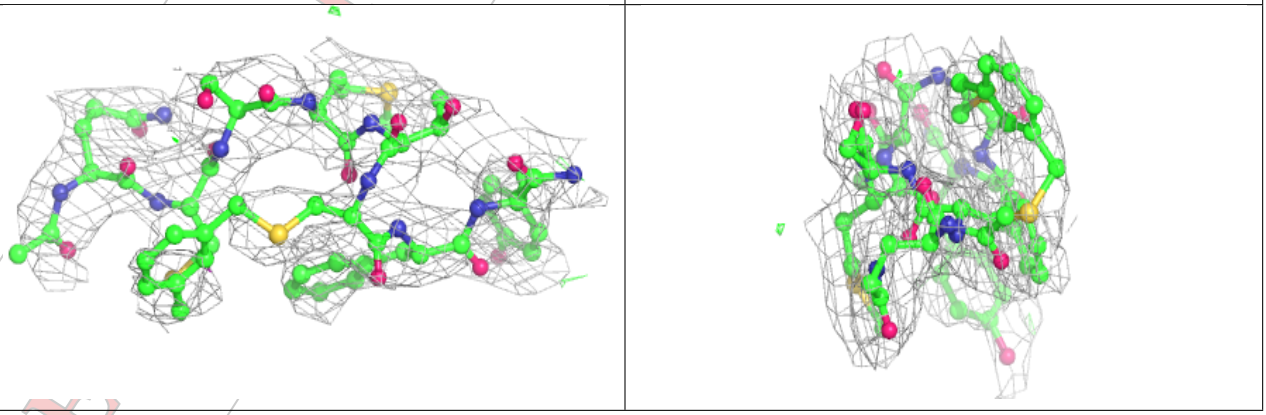




Electron density around LIG D 301:

$2mF_o$-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.