



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2026 – 04:12 am BST

PDB ID : 9QZH / pdb_00009qzh
Title : GID4 in complex with Compound 33
Authors : Pastok, M.W.; Gorecka-Minakowska, K.M.; Klejnot, M.; Skowron, A.N.; Wisniewski, J.; Walczak, M.J.
Deposited on : 2025-04-23
Resolution : 2.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

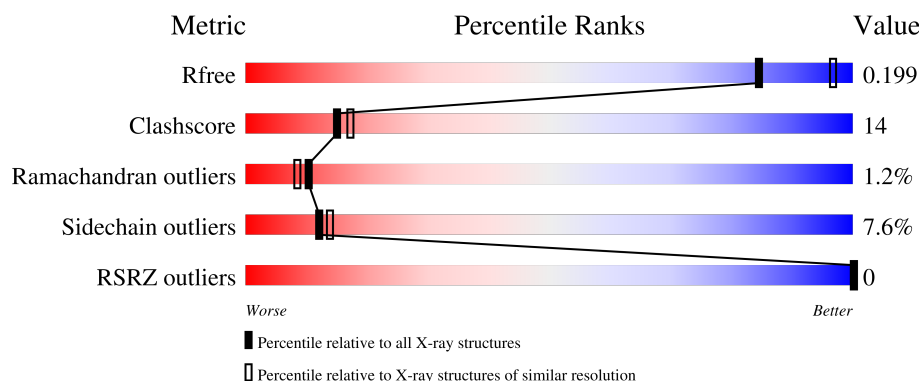
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	166	 65% 21% 8% • 5%
1	B	166	 68% 25% • •
1	C	166	 60% 27% 5% • 7%
1	D	166	 67% 23% • 6%

2 Entry composition [i](#)

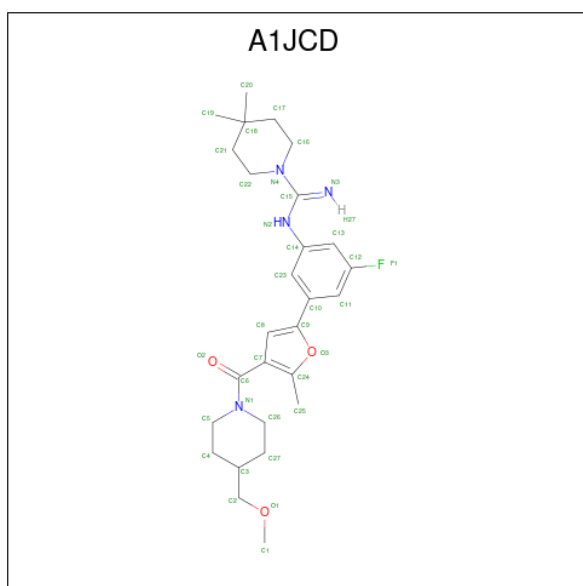
There are 2 unique types of molecules in this entry. The entry contains 5331 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucose-induced degradation protein 4 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1325	862	215	245	3			
1	B	160	Total	C	N	O	S	0	0	0
			1334	865	217	249	3			
1	C	155	Total	C	N	O	S	0	0	0
			1296	842	210	241	3			
1	D	156	Total	C	N	O	S	0	0	0
			1306	847	212	244	3			

- Molecule 2 is {N}-[3-fluoranyl-5-[4-[4-(methoxymethyl)piperidin-1-yl]carbonyl-5-methyl-furan-2-yl]phenyl]-4,4-dimethyl-piperidine-1-carboximidamide (CCD ID: A1JCD) (formula: C₂₇H₃₇FN₄O₃) (labeled as "Ligand of Interest" by depositor).



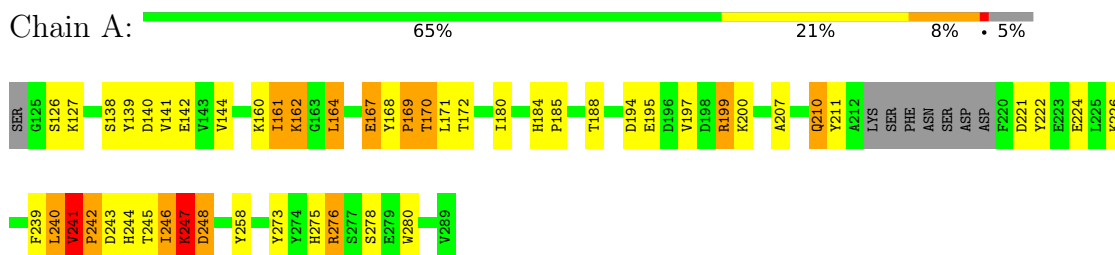
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	3	0
			35	27	1	4	3		

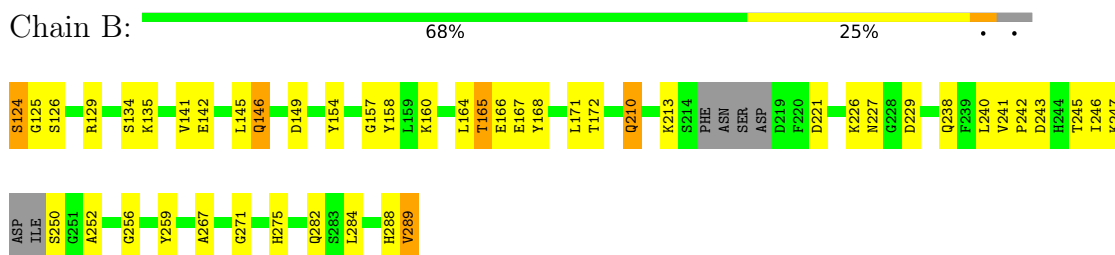
3 Residue-property plots

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.

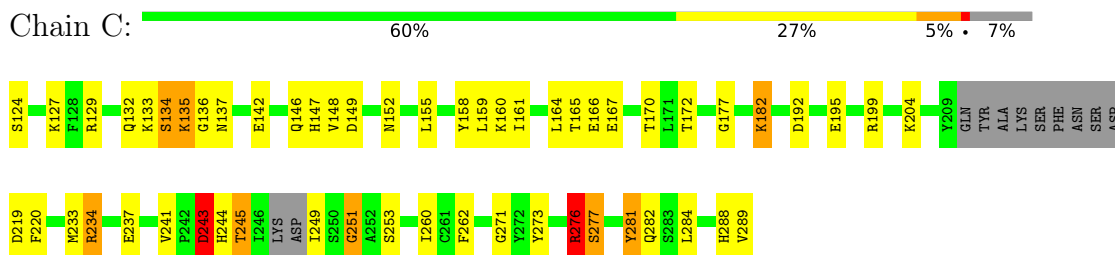
- Molecule 1: Glucose-induced degradation protein 4 homolog



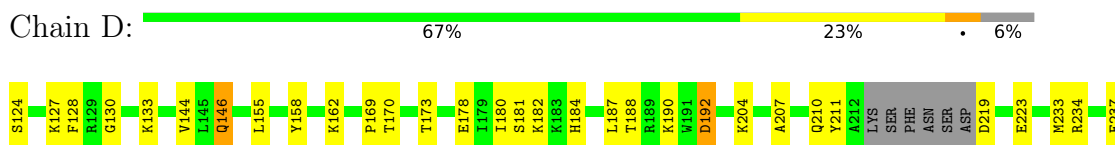
- Molecule 1: Glucose-induced degradation protein 4 homolog



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- Molecule 1: Glucose-induced degradation protein 4 homolog



V241	P242	D243	H244	T245	ILE	LYS	ASP	ILE	S250	G251	A252	S253	Y259	G271	R276	S277	S278	E279	W280	Y281	N285	L286	V289
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 44.46Å 103.06Å 90.00° 112.83° 90.00°	Depositor
Resolution (Å)	47.54 – 2.19 47.54 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.54-2.19) 92.7 (47.54-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.182 , 0.220 0.192 , 0.199	Depositor DCC
R_{free} test set	1787 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5331	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3327e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1JCD

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	0.67	0/1367	1.32	8/1842 (0.4%)
1	B	0.60	0/1375	1.19	4/1851 (0.2%)
1	C	0.67	1/1336 (0.1%)	1.30	6/1799 (0.3%)
1	D	0.68	0/1347	1.31	7/1814 (0.4%)
All	All	0.66	1/5425 (0.0%)	1.28	25/7306 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
1	D	0	3
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	134	SER	CA-CB	-5.22	1.45	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	165	THR	CA-CB-OG1	-7.88	97.77	109.60
1	D	192	ASP	CA-CB-CG	7.72	120.33	112.60
1	A	248	ASP	N-CA-C	-7.16	104.55	113.28
1	D	188	THR	CA-CB-OG1	-6.76	99.46	109.60
1	C	135	LYS	CB-CA-C	6.35	123.06	110.42
1	C	132	GLN	N-CA-CB	-6.06	100.55	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	166	GLU	CB-CG-CD	6.01	122.82	112.60
1	A	211	TYR	CB-CA-C	5.87	119.69	110.19
1	C	262	PHE	N-CA-CB	-5.84	100.53	110.16
1	D	279	GLU	CB-CG-CD	5.67	122.24	112.60
1	D	146	GLN	CB-CA-C	-5.63	100.39	110.70
1	B	284	LEU	N-CA-CB	-5.54	101.38	110.68
1	D	223	GLU	CB-CG-CD	5.46	121.87	112.60
1	A	239	PHE	CA-CB-CG	5.44	119.24	113.80
1	B	146	GLN	CB-CA-C	5.36	119.18	110.24
1	A	243	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	162	LYS	CB-CA-C	5.25	119.41	109.37
1	D	281	TYR	CB-CA-C	-5.20	104.35	111.73
1	C	243	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	188	THR	CA-CB-OG1	-5.18	101.83	109.60
1	B	229	ASP	CB-CA-C	5.16	118.71	110.09
1	D	243	ASP	CA-CB-CG	5.13	117.73	112.60
1	B	149	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	164	LEU	N-CA-CB	5.02	117.29	110.01
1	A	169	PRO	N-CA-C	5.00	120.49	113.53

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	234	ARG	Sidechain
1	C	245	THR	Peptide
1	C	251	GLY	Peptide
1	C	276	ARG	Sidechain
1	D	211	TYR	Peptide
1	D	219	ASP	Peptide
1	D	234	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1325	0	1243	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1334	0	1243	37	0
1	C	1296	0	1212	43	1
1	D	1306	0	1212	22	1
2	C	35	0	0	3	0
2	D	35	0	0	1	0
All	All	5331	0	4910	140	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 14.

All (140) 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:A:246:ILE:O	1:A:247:LYS:C	1.92	1.12
1:A:141:VAL:HG22	1:A:161:ILE:HD13	1.53	0.90
1:A:172:THR:HB	1:A:242:PRO:HD2	1.51	0.90
1:A:276:ARG:HH22	1:B:135:LYS:HB2	1.35	0.90
1:C:149:ASP:OD2	1:C:152:ASN:ND2	2.07	0.88
1:C:276:ARG:HH21	1:C:276:ARG:HG3	1.48	0.78
1:A:162:LYS:HD2	1:A:169:PRO:O	1.86	0.75
1:B:210:GLN:OE1	1:C:147:HIS:HA	1.86	0.75
1:A:246:ILE:O	1:A:248:ASP:N	2.21	0.73
1:A:275:HIS:HB3	1:A:278:SER:OG	1.89	0.73
1:D:155:LEU:HD21	1:D:233:MET:SD	2.30	0.72
1:B:245:THR:HG22	1:B:246:ILE:O	1.89	0.72
1:C:149:ASP:CG	1:C:152:ASN:HD22	1.99	0.70
1:C:134:SER:OG	1:C:134:SER:O	2.07	0.69
1:A:170:THR:O	1:A:171:LEU:HD23	1.94	0.68
1:A:240:LEU:HD23	1:A:247:LYS:HB2	1.75	0.68
1:A:127:LYS:HG3	1:A:144:VAL:HG22	1.74	0.68
1:D:127:LYS:O	1:D:289:VAL:HG23	1.92	0.68
1:A:185:PRO:HB3	1:A:222:TYR:OH	1.94	0.68
1:D:124:SER:OG	1:D:144:VAL:HG11	1.94	0.67
1:C:164:LEU:HD22	1:C:164:LEU:H	1.59	0.67
1:A:127:LYS:HE3	1:A:142:GLU:OE1	1.95	0.66
1:C:192:ASP:OD2	1:C:276:ARG:NE	2.29	0.65
1:B:134:SER:HA	1:B:282:GLN:HE21	1.61	0.64
1:C:276:ARG:HG3	1:C:276:ARG:NH2	2.11	0.64
1:A:195:GLU:OE2	1:A:199:ARG:NH1	2.31	0.64
1:B:134:SER:OG	1:B:282:GLN:NE2	2.31	0.64
1:B:238:GLN:HA	1:B:238:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LYS:H	1:C:182:LYS:HE2	1.62	0.63
1:A:241:VAL:HB	1:A:242:PRO:HD3	1.80	0.62
1:D:204:LYS:HD2	1:D:281:TYR:CE1	2.37	0.60
1:A:172:THR:CB	1:A:242:PRO:HD2	2.29	0.60
1:B:246:ILE:O	1:B:247:LYS:CB	2.51	0.58
1:B:160:LYS:HG3	1:B:172:THR:OG1	2.02	0.58
1:D:128:PHE:HB3	1:D:286:LEU:HB3	1.86	0.58
1:A:247:LYS:NZ	1:A:247:LYS:HB3	2.19	0.57
1:B:267:ALA:HB1	1:B:288:HIS:HB2	1.87	0.57
1:D:178:GLU:OE2	1:D:190:LYS:NZ	2.31	0.56
1:B:164:LEU:O	1:B:165:THR:HB	2.06	0.56
1:B:288:HIS:CE1	1:B:289:VAL:OXT	2.58	0.56
1:A:172:THR:HB	1:A:242:PRO:CD	2.30	0.56
1:B:167:GLU:O	1:B:168:TYR:CD2	2.59	0.56
1:B:227:ASN:HD22	1:D:133:LYS:NZ	2.03	0.55
1:A:241:VAL:CB	1:A:242:PRO:HD3	2.37	0.55
1:B:246:ILE:O	1:B:247:LYS:HG3	2.08	0.54
1:C:204:LYS:HD2	1:C:281:TYR:CD1	2.43	0.54
1:D:204:LYS:HD2	1:D:281:TYR:CD1	2.42	0.54
1:C:177:GLY:HA2	1:C:234:ARG:O	2.08	0.54
1:B:246:ILE:O	1:B:247:LYS:HB2	2.06	0.54
1:A:161:ILE:HD12	1:A:162:LYS:H	1.73	0.53
1:C:149:ASP:CG	1:C:152:ASN:ND2	2.63	0.53
1:A:200:LYS:HD3	1:A:280:TRP:CZ3	2.44	0.53
1:C:249:ILE:CD1	1:C:253:SER:HB2	2.39	0.52
1:C:243:ASP:HB3	1:C:244:HIS:CD2	2.45	0.52
1:C:204:LYS:HD2	1:C:281:TYR:CE1	2.44	0.52
1:D:237:GLU:OE2	2:D:301:A1JCD:N2	2.43	0.52
1:C:160:LYS:HG2	1:C:172:THR:OG1	2.09	0.52
1:C:127:LYS:HD2	1:C:142:GLU:OE2	2.10	0.52
1:A:246:ILE:O	1:A:247:LYS:O	2.24	0.51
1:B:165:THR:OG1	1:B:167:GLU:CD	2.53	0.51
1:A:139:TYR:CB	1:A:161:ILE:HD11	2.40	0.51
1:D:207:ALA:O	1:D:210:GLN:HB3	2.10	0.51
1:A:247:LYS:O	1:A:247:LYS:HG2	2.11	0.50
1:C:136:GLY:O	1:C:137:ASN:ND2	2.44	0.49
1:C:237:GLU:OE1	2:C:301:A1JCD:N3	2.44	0.49
1:B:134:SER:CA	1:B:282:GLN:HE21	2.25	0.49
1:C:134:SER:O	1:C:135:LYS:CB	2.60	0.49
1:A:246:ILE:C	1:A:248:ASP:N	2.70	0.48
1:B:165:THR:CG2	1:B:168:TYR:HB2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:SER:HB3	2:C:301:A1JCD:C8	2.43	0.48
1:A:221:ASP:OD1	1:A:224:GLU:HB2	2.13	0.48
1:A:242:PRO:O	1:A:244:HIS:CE1	2.66	0.48
1:C:276:ARG:HH21	1:C:276:ARG:CG	2.22	0.48
1:A:200:LYS:HD3	1:A:280:TRP:HZ3	1.79	0.48
1:A:140:ASP:O	1:A:161:ILE:HD12	2.14	0.48
1:C:161:ILE:HG23	1:C:164:LEU:HD21	1.96	0.48
1:C:195:GLU:HG2	1:C:199:ARG:HD2	1.96	0.47
1:B:241:VAL:O	1:B:242:PRO:C	2.58	0.47
1:C:134:SER:O	1:C:135:LYS:HB3	2.14	0.47
1:B:129:ARG:NH1	1:B:289:VAL:HG11	2.30	0.47
1:B:259:TYR:O	1:B:271:GLY:HA2	2.15	0.47
1:D:251:GLY:C	1:D:253:SER:H	2.22	0.46
1:A:139:TYR:HB2	1:A:161:ILE:HD11	1.97	0.46
1:B:210:GLN:OE1	1:C:148:VAL:N	2.48	0.46
1:A:161:ILE:HD12	1:A:162:LYS:N	2.31	0.45
1:C:155:LEU:HD21	1:C:177:GLY:HA3	1.98	0.45
1:D:259:TYR:O	1:D:271:GLY:HA2	2.17	0.45
1:B:165:THR:HG23	1:B:168:TYR:HB2	1.98	0.45
1:B:168:TYR:HB3	1:B:171:LEU:HD21	1.99	0.45
1:B:146:GLN:HB2	1:B:157:GLY:HA2	1.97	0.45
1:D:276:ARG:HG3	1:D:277:SER:N	2.32	0.45
1:B:134:SER:CB	1:B:282:GLN:HE21	2.30	0.45
1:C:129:ARG:NH1	1:C:289:VAL:HG21	2.31	0.45
1:D:146:GLN:HG3	1:D:158:TYR:CE2	2.51	0.45
1:A:171:LEU:HA	1:A:244:HIS:CE1	2.51	0.44
1:A:194:ASP:OD1	1:A:197:VAL:HG23	2.17	0.44
1:A:276:ARG:HH22	1:B:135:LYS:CB	2.19	0.44
1:C:249:ILE:HG13	1:C:251:GLY:H	1.82	0.44
1:B:164:LEU:O	1:B:165:THR:CB	2.62	0.44
1:D:158:TYR:HA	1:D:173:THR:O	2.17	0.44
1:B:164:LEU:HD12	1:B:171:LEU:HD12	1.99	0.44
1:D:187:LEU:HD12	1:D:187:LEU:HA	1.89	0.44
1:C:136:GLY:C	1:C:137:ASN:ND2	2.76	0.44
1:A:168:TYR:N	1:A:169:PRO:HD3	2.33	0.43
1:D:180:ILE:HA	1:D:184:HIS:O	2.18	0.43
1:B:246:ILE:O	1:B:247:LYS:CG	2.66	0.43
1:C:273:TYR:CE1	2:C:301:A1JCD:N3	2.86	0.43
1:A:168:TYR:OH	1:A:248:ASP:HB3	2.17	0.43
1:A:241:VAL:HB	1:A:242:PRO:CD	2.48	0.43
1:C:158:TYR:HE1	1:C:241:VAL:HG21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:H	1:C:164:LEU:CD2	2.30	0.43
1:C:133:LYS:HA	1:C:137:ASN:O	2.18	0.43
1:B:124:SER:OG	1:B:125:GLY:N	2.50	0.43
1:C:159:LEU:O	1:C:172:THR:HA	2.19	0.43
1:A:207:ALA:O	1:A:210:GLN:HB2	2.19	0.42
1:A:246:ILE:CG2	1:A:247:LYS:N	2.83	0.42
1:B:146:GLN:HG3	1:B:158:TYR:CE2	2.54	0.42
1:D:181:SER:O	1:D:182:LYS:C	2.61	0.42
1:A:139:TYR:HB3	1:A:161:ILE:HD11	2.00	0.42
1:C:288:HIS:HD2	1:C:289:VAL:N	2.18	0.42
1:C:134:SER:OG	1:C:282:GLN:NE2	2.53	0.42
1:C:249:ILE:HD12	1:C:253:SER:CB	2.50	0.42
1:C:271:GLY:N	1:C:284:LEU:O	2.49	0.42
1:D:130:GLY:HA3	1:D:285:ASN:O	2.19	0.42
1:A:240:LEU:CD2	1:A:247:LYS:HA	2.50	0.42
1:B:256:GLY:CA	1:B:275:HIS:HD2	2.33	0.41
1:A:167:GLU:C	1:A:169:PRO:HD3	2.45	0.41
1:B:125:GLY:HA3	1:B:145:LEU:O	2.20	0.41
1:A:180:ILE:HA	1:A:184:HIS:O	2.19	0.41
1:C:276:ARG:HD3	1:C:277:SER:OG	2.21	0.41
1:A:245:THR:O	1:A:246:ILE:C	2.62	0.41
1:B:154:TYR:CD1	1:B:154:TYR:C	2.98	0.41
1:D:127:LYS:C	1:D:289:VAL:HG23	2.46	0.41
1:C:158:TYR:CE1	1:C:241:VAL:HG21	2.56	0.41
1:D:127:LYS:HB3	1:D:289:VAL:CG2	2.51	0.41
1:C:192:ASP:OD2	1:C:276:ARG:CZ	2.69	0.41
1:C:233:MET:HB2	1:C:260:ILE:HB	2.02	0.40
1:B:141:VAL:HG12	1:B:142:GLU:N	2.35	0.40
1:B:227:ASN:HB2	1:D:133:LYS:HZ1	1.86	0.40
1:A:258:TYR:CE2	1:A:273:TYR:HB2	2.56	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)
1:C:167:GLU:OE1	1:D:279:GLU:OE2[2_657]	2.11	0.09

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	154/166 (93%)	140 (91%)	11 (7%)	3 (2%)	6	4
1	B	154/166 (93%)	138 (90%)	14 (9%)	2 (1%)	9	8
1	C	149/166 (90%)	140 (94%)	8 (5%)	1 (1%)	18	19
1	D	150/166 (90%)	140 (93%)	9 (6%)	1 (1%)	18	19
All	All	607/664 (91%)	558 (92%)	42 (7%)	7 (1%)	10	8

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	VAL
1	A	242	PRO
1	A	247	LYS
1	B	243	ASP
1	B	252	ALA
1	C	281	TYR
1	D	169	PRO

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	139/147 (95%)	124 (89%)	15 (11%)	6	6
1	B	140/147 (95%)	129 (92%)	11 (8%)	11	13
1	C	137/147 (93%)	127 (93%)	10 (7%)	13	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	137/147 (93%)	131 (96%)	6 (4%)	25	34
All	All	553/588 (94%)	511 (92%)	42 (8%)	12	14

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	SER
1	A	138	SER
1	A	160	LYS
1	A	161	ILE
1	A	164	LEU
1	A	167	GLU
1	A	170	THR
1	A	199	ARG
1	A	210	GLN
1	A	226	LYS
1	A	240	LEU
1	A	241	VAL
1	A	246	ILE
1	A	247	LYS
1	A	276	ARG
1	B	124	SER
1	B	126	SER
1	B	165	THR
1	B	166	GLU
1	B	210	GLN
1	B	213	LYS
1	B	221	ASP
1	B	226	LYS
1	B	240	LEU
1	B	250	SER
1	B	289	VAL
1	C	124	SER
1	C	146	GLN
1	C	170	THR
1	C	182	LYS
1	C	219	ASP
1	C	220	PHE
1	C	243	ASP
1	C	245	THR
1	C	276	ARG
1	C	277	SER

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Mol	Chain	Res	Type
1	D	162	LYS
1	D	170	THR
1	D	192	ASP
1	D	241	VAL
1	D	243	ASP
1	D	253	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	227	ASN
1	A	244	HIS
1	A	263	GLN
1	B	132	GLN
1	B	227	ASN
1	B	275	HIS
1	B	282	GLN
1	C	137	ASN
1	C	152	ASN
1	C	244	HIS
1	C	282	GLN
1	C	288	HIS
1	D	132	GLN
1	D	244	HIS
1	D	275	HIS
1	D	282	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	A1JCD	C	301	-	37,38,38	1.54	2 (5%)	49,55,55	1.33	6 (12%)
2	A1JCD	D	301	-	37,38,38	1.21	1 (2%)	49,55,55	1.18	4 (8%)

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	A1JCD	C	301	-	-	5/23/45/45	0/4/4/4
2	A1JCD	D	301	-	-	6/23/45/45	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1JCD	C15-N2	-8.53	1.27	1.37
2	D	301	A1JCD	C15-N2	-6.90	1.29	1.37
2	C	301	A1JCD	O1-C2	2.47	1.51	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	A1JCD	C7-C6-N1	4.34	123.66	118.74
2	D	301	A1JCD	N4-C15-N3	-3.17	113.74	121.23
2	D	301	A1JCD	N2-C15-N4	3.00	123.36	117.45
2	C	301	A1JCD	C26-N1-C5	2.64	117.71	112.62
2	C	301	A1JCD	C4-C3-C2	2.63	117.88	111.28
2	D	301	A1JCD	C21-C22-N4	2.53	115.93	110.92
2	C	301	A1JCD	C21-C18-C17	2.50	112.13	108.71
2	C	301	A1JCD	O2-C6-N1	-2.42	118.82	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	A1JCD	C27-C26-N1	2.20	114.17	110.82
2	C	301	A1JCD	C21-C22-N4	2.09	115.04	110.92

There are no chirality outliers.

All (11) torsion outliers are listed below:

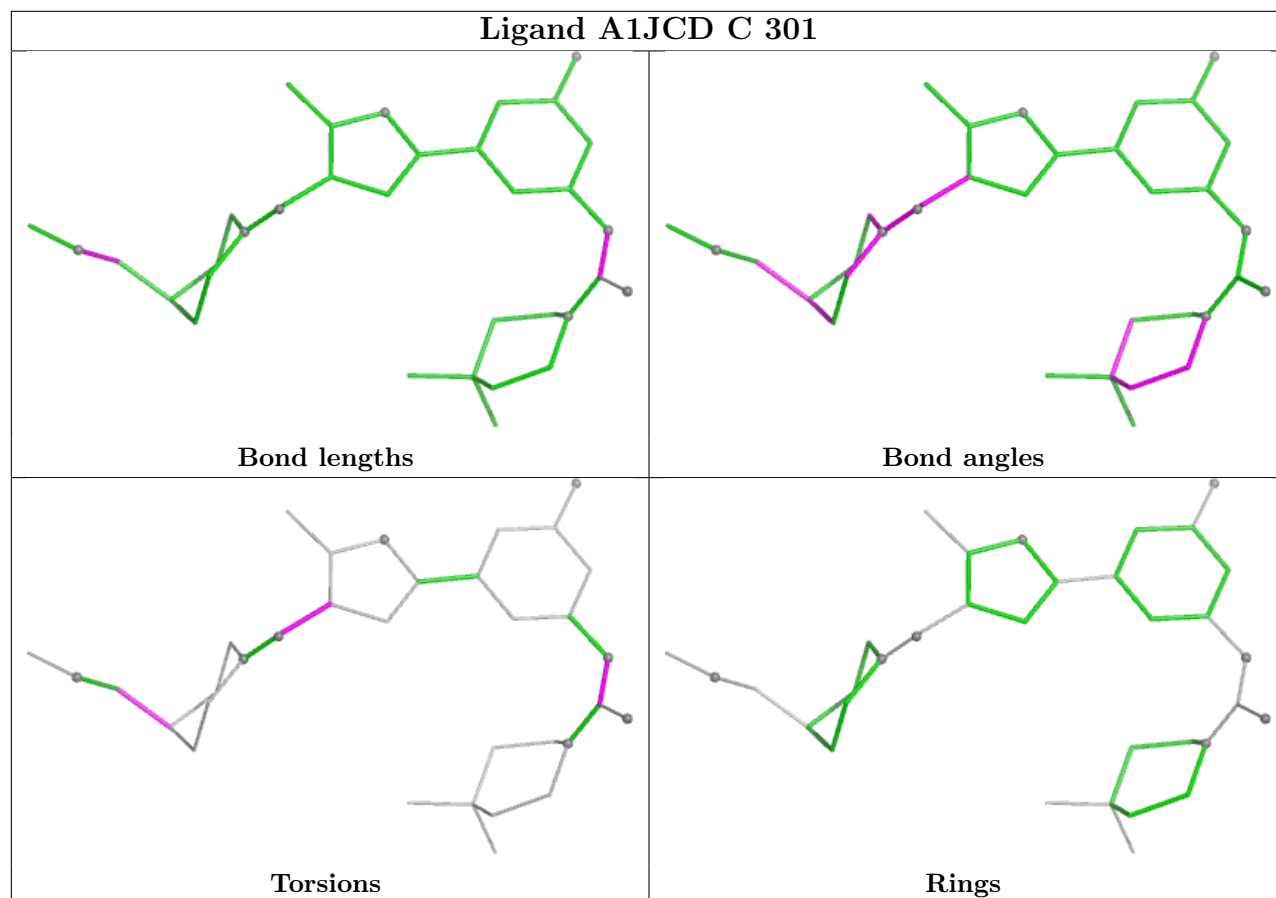
Mol	Chain	Res	Type	Atoms
2	C	301	A1JCD	O1-C2-C3-C27
2	C	301	A1JCD	N3-C15-N2-C14
2	C	301	A1JCD	N4-C15-N2-C14
2	D	301	A1JCD	N1-C6-C7-C8
2	D	301	A1JCD	O2-C6-C7-C8
2	D	301	A1JCD	N3-C15-N4-C16
2	D	301	A1JCD	N3-C15-N4-C22
2	C	301	A1JCD	O1-C2-C3-C4
2	D	301	A1JCD	N2-C15-N4-C22
2	C	301	A1JCD	O2-C6-C7-C8
2	D	301	A1JCD	N3-C15-N2-C14

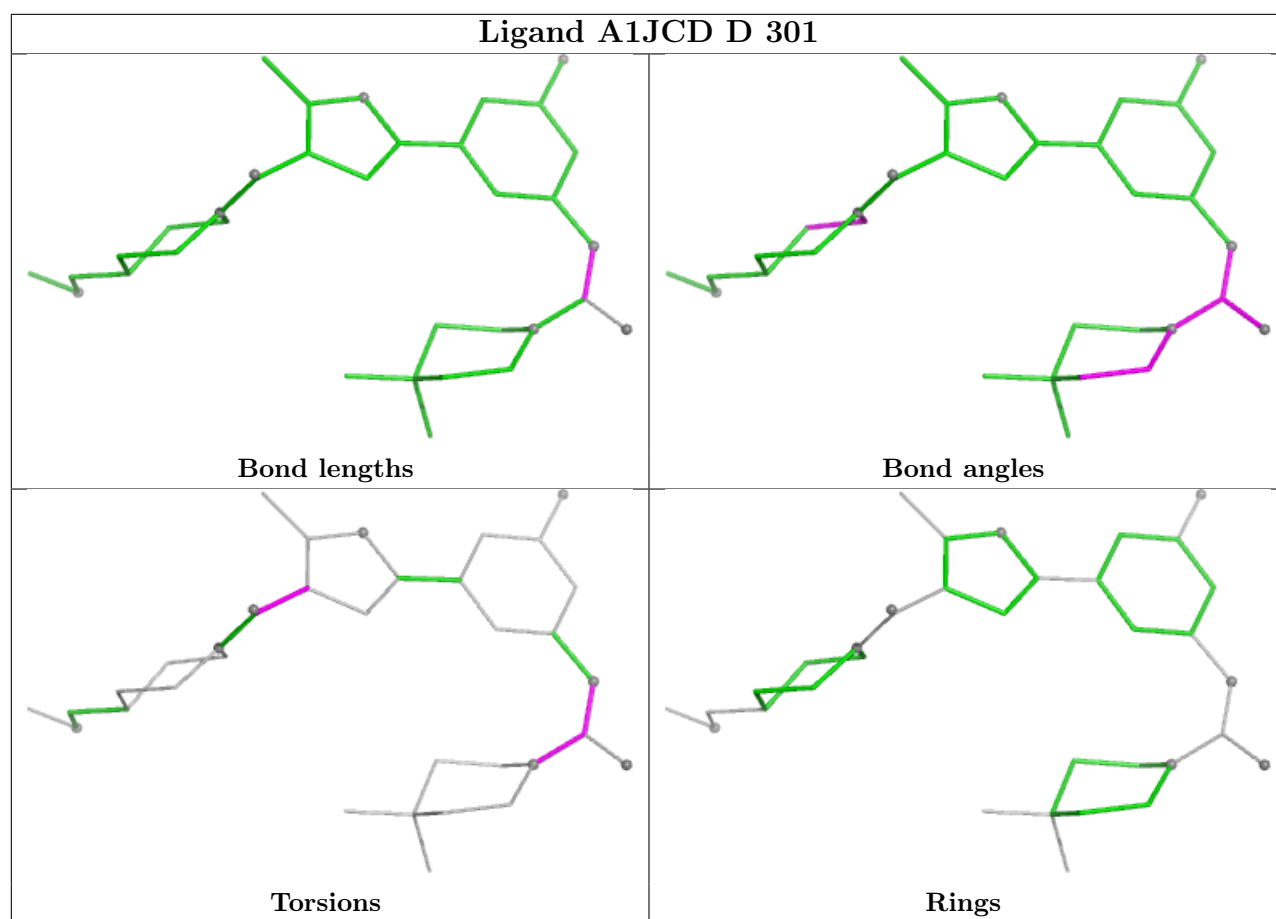
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	A1JCD	3	0
2	D	301	A1JCD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	158/166 (95%)	-1.39	0 100 100	23, 36, 55, 72	0
1	B	160/166 (96%)	-1.28	0 100 100	26, 42, 60, 78	0
1	C	155/166 (93%)	-1.33	0 100 100	24, 37, 60, 77	0
1	D	156/166 (93%)	-1.40	0 100 100	22, 34, 53, 72	0
All	All	629/664 (94%)	-1.35	0 100 100	22, 37, 56, 78	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

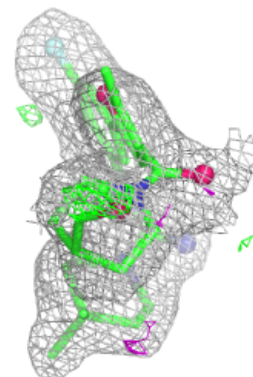
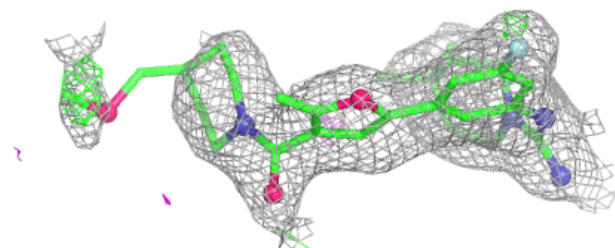
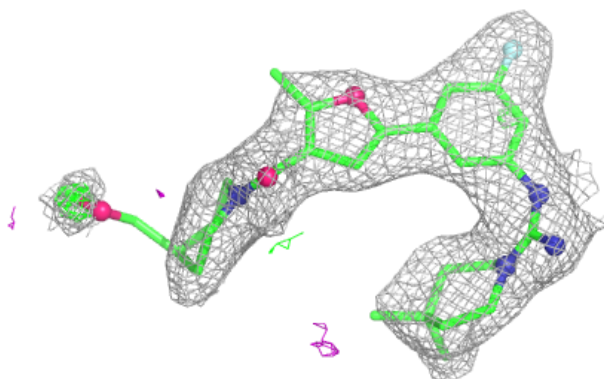
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1JCD	C	301	35/35	0.99	0.03	19,40,52,55	3
2	A1JCD	D	301	35/35	0.99	0.03	25,37,56,58	3

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.

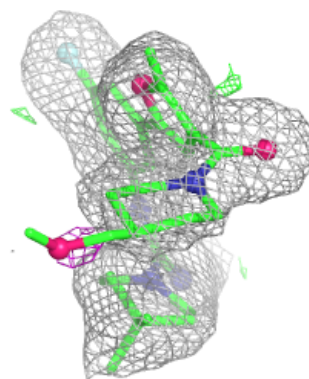
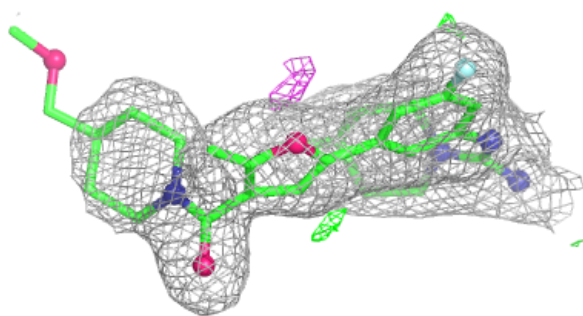
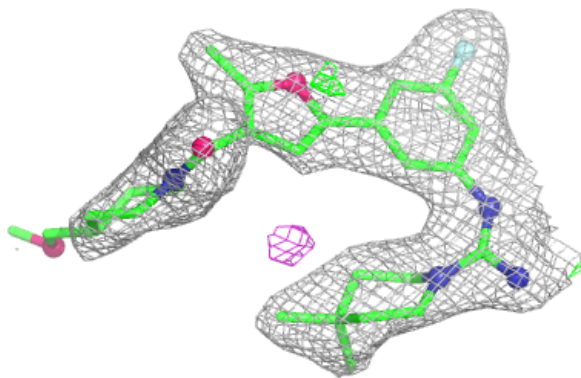
Electron density around A1JCD C 301:

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



Electron density around A1JCD 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 ⓘ

There are no such residues in this entry.