



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:29 AM UTC

PDB ID : 4YFK / pdb_00004yfk
Title : Escherichia coli RNA polymerase in complex with squaramide compound 8.
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.;
McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.57 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

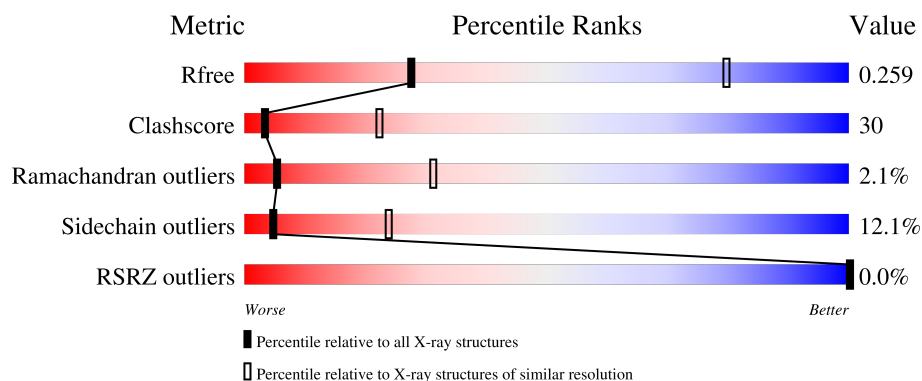
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	329	35% 45% 16% ••
1	B	329	27% 31% 7% • 34%
1	G	329	30% 32% 7% 31%
1	H	329	25% 34% 6% 34%
2	C	1342	44% 46% 9% •

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55782 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9050	5690	1620	1694	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8990	5654	1608	1682	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

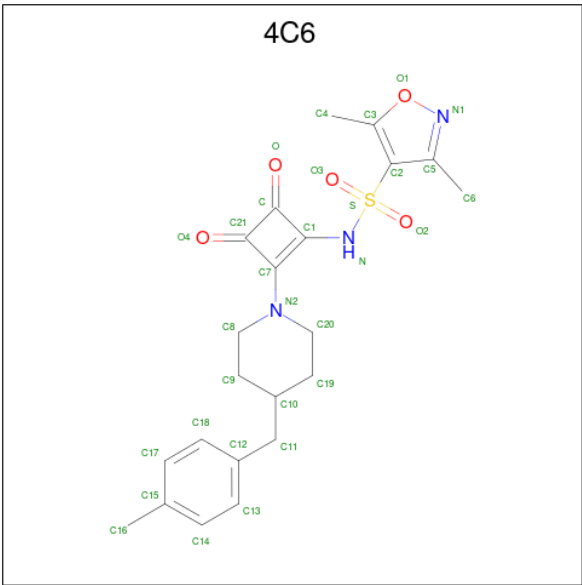
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	2	Total	Zn	0	0
			2	2		

- Molecule 8 is 3,5-dimethyl-N-{2-[4-(4-methylbenzyl)piperidin-1-yl]-3,4-dioxocyclobut-1-en-1-yl}-1,2-oxazole-4-sulfonamide (CCD ID: 4C6) (formula: C₂₂H₂₅N₃O₅S).

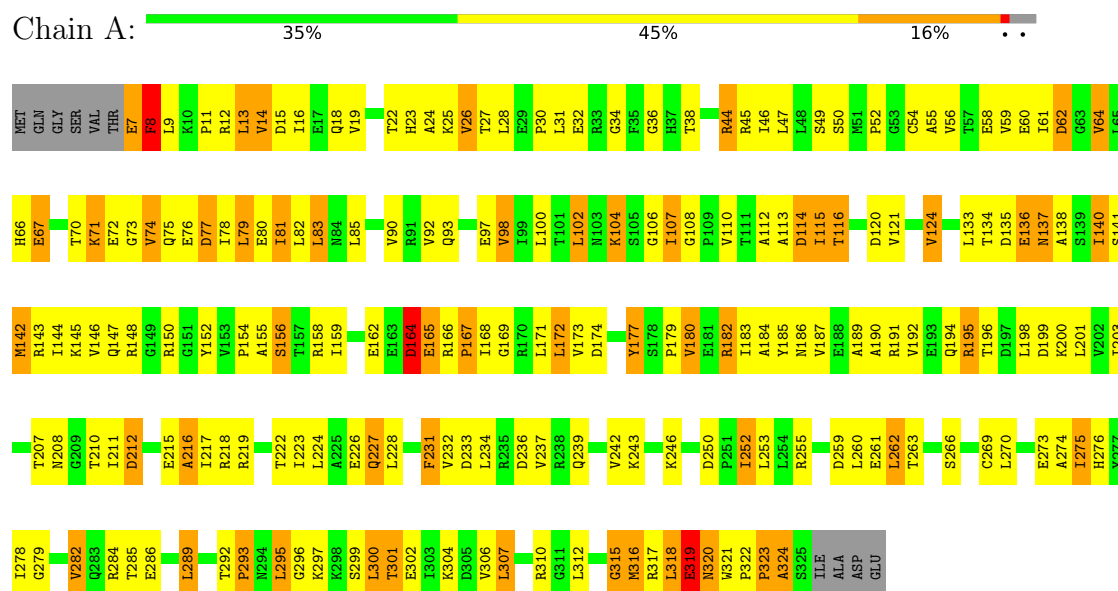


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	N	O	S	0	0
			31	22	3	5	1		
8	J	1	Total	C	N	O	S	0	0
			31	22	3	5	1		

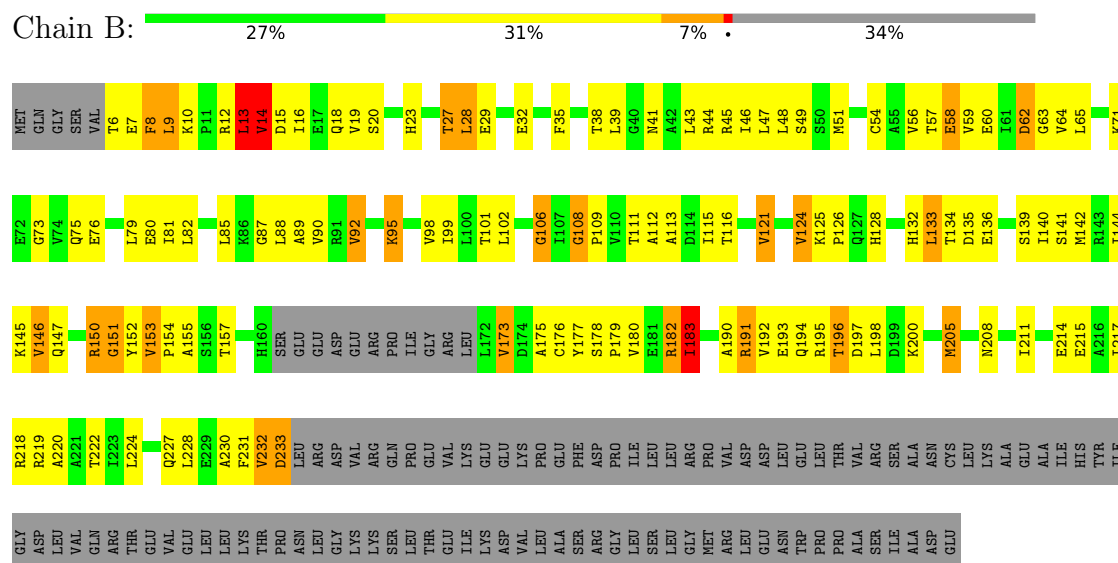
3 Residue-property plots

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.

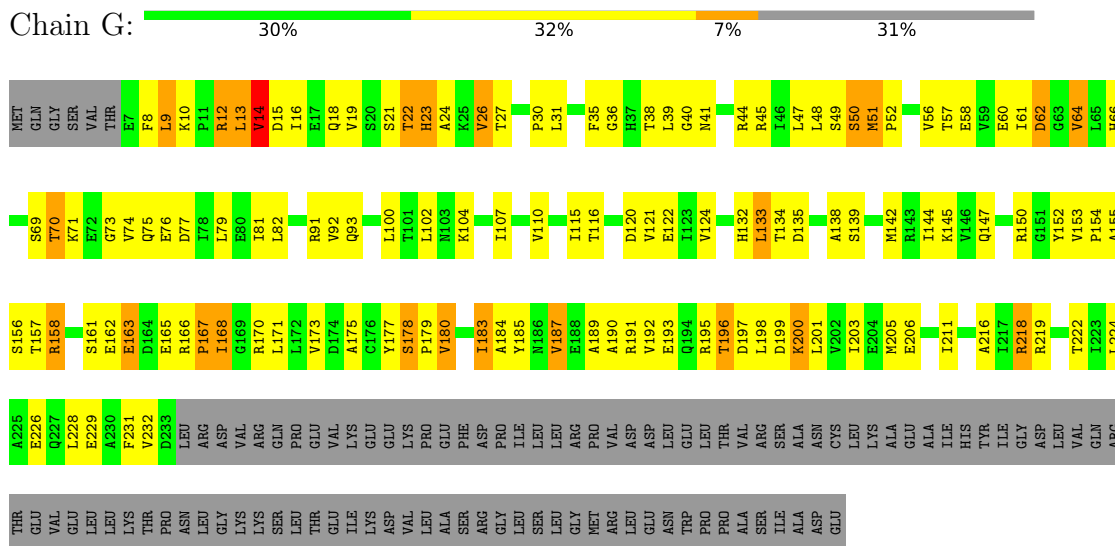
• Molecule 1: DNA-directed RNA polymerase subunit alpha



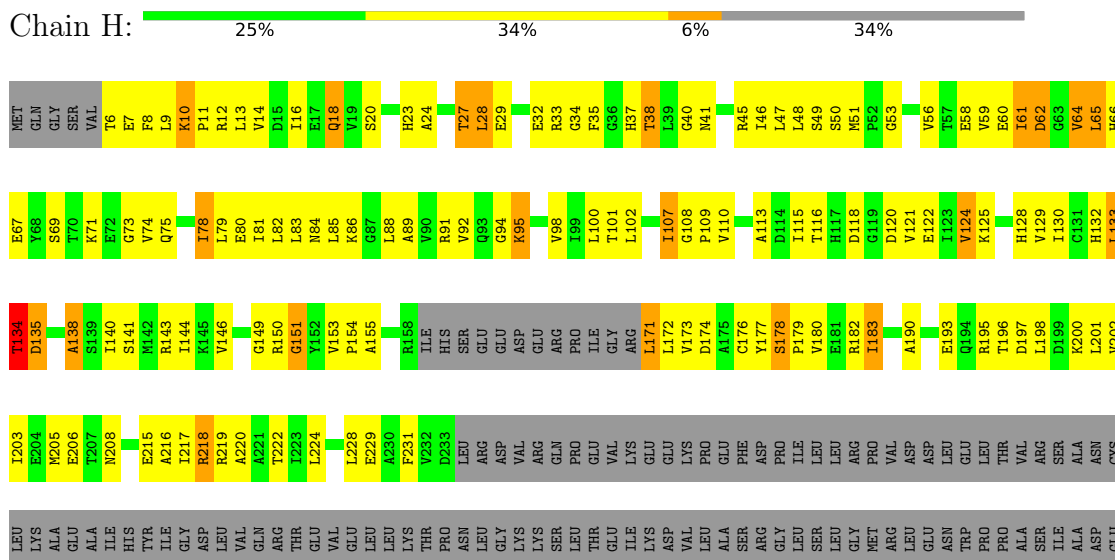
• Molecule 1: DNA-directed RNA polymerase subunit alpha



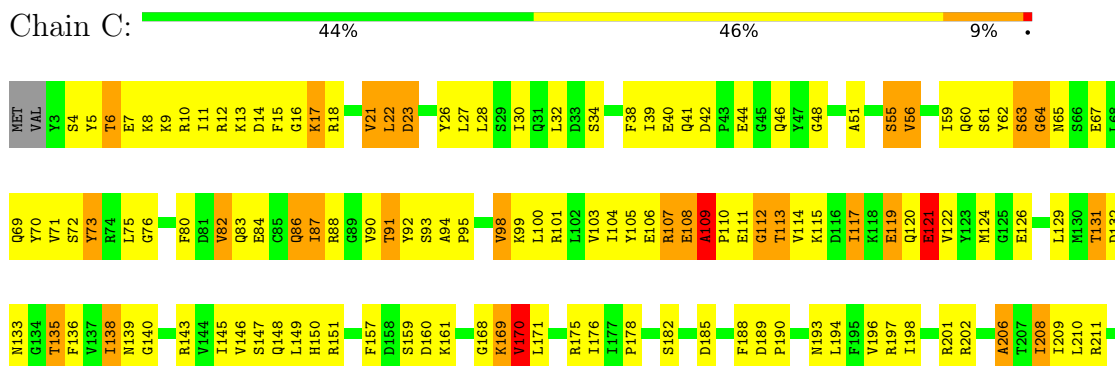
• Molecule 1: DNA-directed RNA polymerase subunit alpha

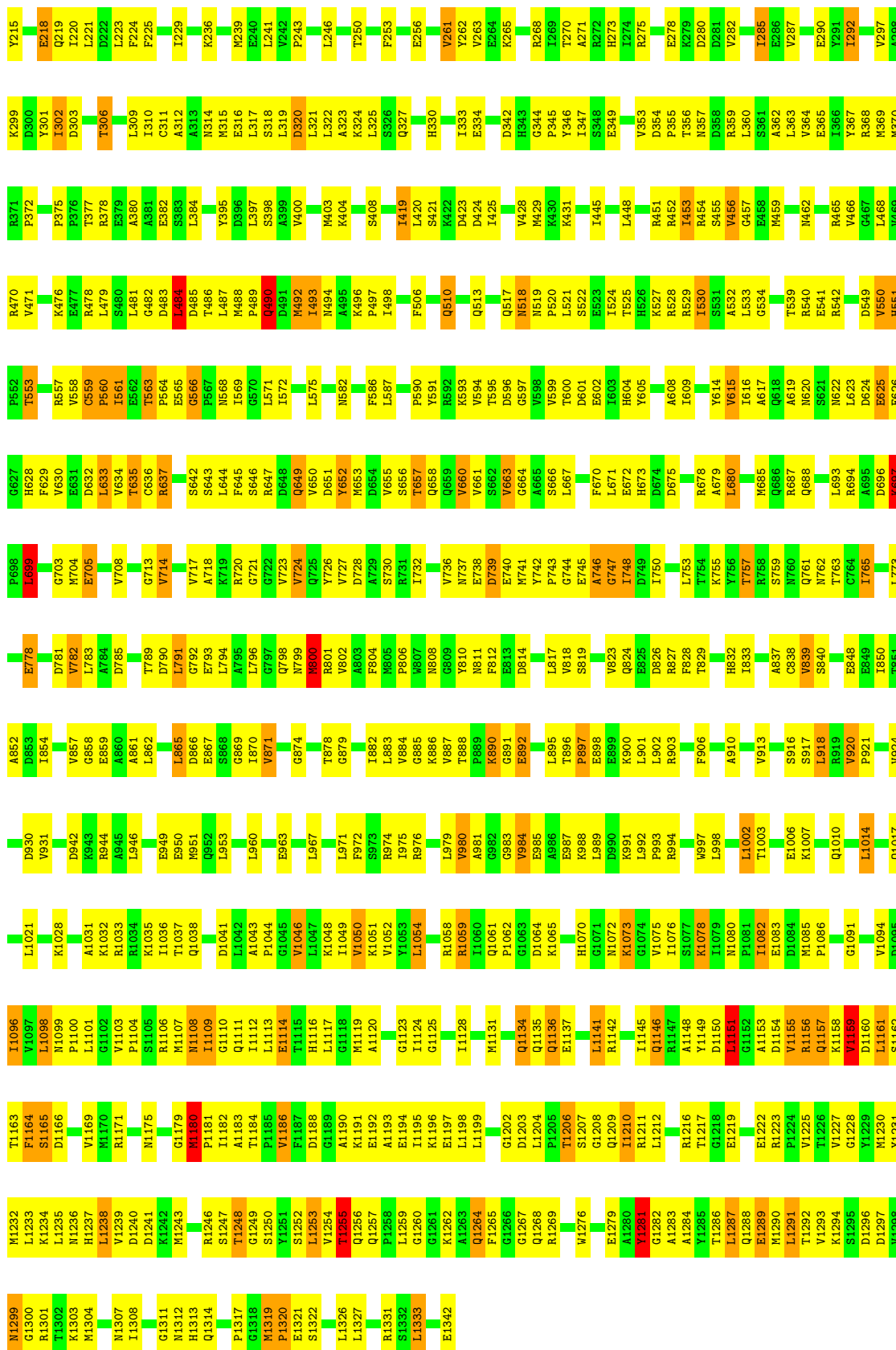


• Molecule 1: DNA-directed RNA polymerase subunit alpha

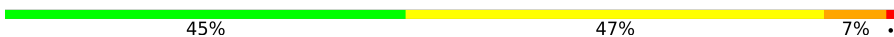


• Molecule 2: DNA-directed RNA polymerase subunit beta

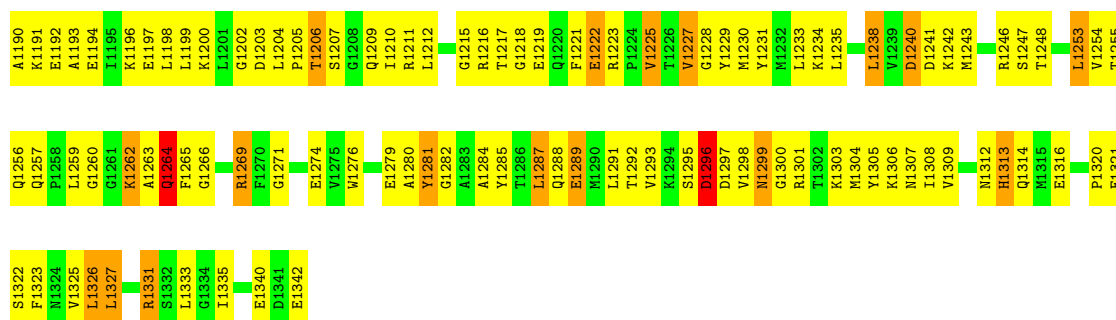




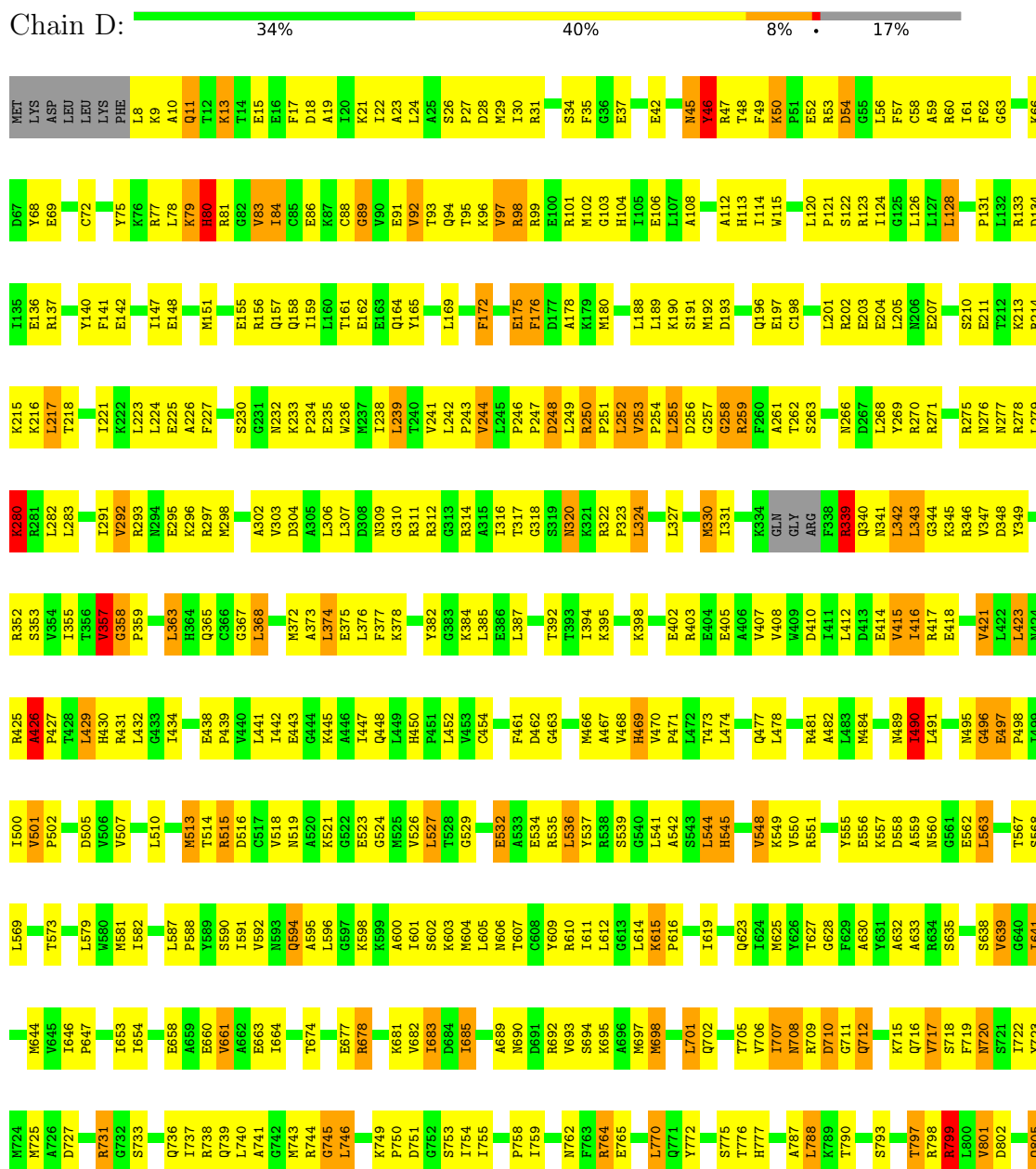
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:  45% 47% 7%

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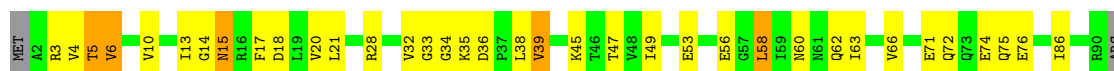
• Molecule 3: DNA-directed RNA polymerase subunit beta'



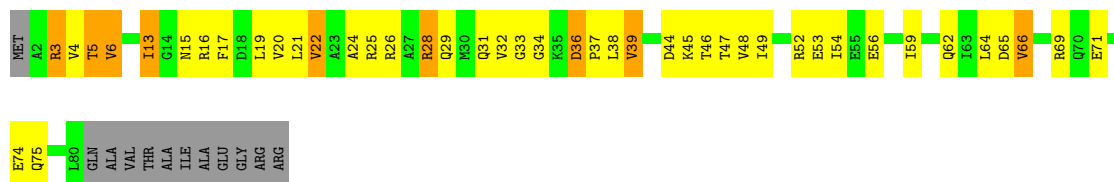
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SER	L1306	I1233	E1188	ASP	PHE	VAL	I908	V831	L746	M680	K599	C517	K445	K370
LEU	ALA	I1234	E1189	MET	VAL	ILE	I909	V832	A748	K681	A600	V518	Q448	L374
LEU	LEU	M1235	I1182	PRO	ARG	THR	N910	K832	A749	V682	I601	N519	L449	E375
LEU	LEU	E1236	V1183	GLN	PHE	THR	K911	E833	P750	I683	S602	K520	H450	L376
ASN	LEU	V1237	S1184	TYR	ASP	ASN	G912	P834	D751	D684	K603	A521	P451	
ASN	ALA	Q1238	F1185	PHE	MET	THR	I915	L835	G752	I685	M604	G522	L452	P379
ALA	ALA	G1166	G1186	LEU	ILE	GLU	G916	V839	S753	A689	L605	M525	A459	F380
GLY	GLY	K1167	K1168	ASP	ASP	LEU	V917	R842	I754	M690	Y609	V527	I381	I381
GLY	GLY	E1168	E1169	GLN	GLN	LYS	I918	R843	P758	D691	R610	L527	G383	G383
GLY	ALA	K1170	T1169	LEU	THR	ILE	I923	T844	A761	R692	I611	T528	D462	K384
SER	ILE	G1171	G1172	ASP	ILE	ASP	G924	A845	N768	V693	L612	E532	D464	L385
ASP	VAL	K1172	R1173	THR	THR	GLU	P925	E846	N762	S694	G613		Q465	
ASN	GLN	R1174	R1175	ARG	ARG	PHE	P926	D847	F763	K695	L614		D466	
GLU	GLN	L1175	L1176	GLN	GLN	GLY		V848	R764	M697	P616		M466	
LEU	LEU	L1176	L1177	THR	THR	ARG	L930	L849	F772	M698			V468	
ASP	ASP	V1176	T1177	ASP	ASP	THR	T931	K850	L767	D699	I619		H469	
GLY	GLY	I1177	I1178	GLU	GLU	LYS	MET	P851	N768	N700	F620		V470	
VAL	VAL	T1178	T1179	LEU	LEU	GLU	ARG	G852	N769	L701			P471	
GLN	GLN	P1179	V1180	THR	THR	THR	THR	T853	L770	Q702	Q623		L472	
ILE	ILE	V1180	D1181	GLY	GLY	TYR	PHE	A854	Q771	T703	I624		T473	
SER	SER	G1182	G1183	LEU	LEU	VAL	HIS	D855	F772	E704	M625		L474	
GLY	GLY	S1183	S1184	SER	SER	PRO	ILE	T856	F773	T705			E475	
ASP	ASP	D1184	D1185	LEU	LEU	TYR	GLY	L857	I774	V706	G628		A476	
THR	THR	P1185	P1186	VAL	VAL	GLY	ALA	P858	S775	I707			Q477	
ALA	ALA	Y1186	Y1187	VAL	VAL	ALA	ALA	R860	T776	N708	Y631		L478	
ARG	ARG	M1189	M1190	ALA	ASP	LEU	ARG	R861	H777	R709	R634		E479	
ILE	ILE	K1192	K1193	PRO	SER	ALA	ALA	T862	R780	G711	S635		R481	
PRO	PRO	V1193	V1194	GLN	ALA	LYS	ALA	L863	L788	Q712	G636		A482	
GLN	GLN	L1195	L1196	GLU	GLU	GLY	ALA	R865		Q716	A637		L483	
SER	SER	Q1195	Q1196	THR	THR	ASP	ALA	E866	S793	V717	S638		M484	
GLY	GLY	L1196	L1197	ALA	ALA	GLY	SER	Q867		S718	V639		M485	
THR	THR	F1199	F1200	GLY	GLY	GLN	ILE	L796	L796	F719	I641		S486	
LYS	LYS	E1202	E1203	THR	GLY	VAL	ILE	T937	T937	N720			M488	
ILE	ILE	R1203	R1204	ASP	LYS	ALA	VAL	R795	R799	S721	M644		M489	
THR	THR	V1205	V1206	THR	ASP	LEU	VAL	V894	L800	I722	V645		I490	
GLY	GLY	G1137	G1138	GLY	PRO	ARG	GLY	S884	V801	M724	I646		P420	
ALA	ALA	L1138	L1139	ALA	ALA	THR	SER	V885	B802	M725	E648		V421	
LEU	LEU	P1139	P1140	LEU	VAL	VAL	ILE		A804		K649		L423	
ILE	ILE	R1140	R1141	ILE	VAL	THR	LEU		Q805		K650		M424	
ASP	ASP	E1146	E1147	ASP	VAL	ASP	LEU	C895	D806		I654		R425	
ALA	ALA	R1148	R1149	ALA	ASP	PRO	ASN	A896	V809	S733	A657		I500	
GLN	GLN	P1150	P1151	GLN	GLN	HIS	VAL	H897	T810	A734	S503		Q504	
ASN	ASN	F1152	F1153	ASN	THR	THR	LYS	C898	E811	A735	E658		D505	
ALA	ALA	L1154	L1155	ALA	MET	PRO	LYS	V899	D812	Q736	A659		V506	
THR	THR	R1222	R1223	THR	ASP	VAL	VAL	G900	D813	I737	E660		L432	
ALA	ALA	V1226	V1227	ALA	VAL	ILE	ASN	R901	H817	R738	V661		L510	
GLU	GLU	T1301	T1302	GLU	LEU	THR	SER	D902	L740	Q739	I591		Y511	
ASP	ASP	R1304	R1305	ASP	ILE	GLU	SER	L903	I820	A741	I664		Y512	
SER	SER			SER	PRO	VAL	GLY	A904	V825	G742	T674		M513	
					GLY	SER	LYS	R905	I826	M743	L596		T514	
								G906		R744	R678		E443	

● Molecule 4: DNA-directed RNA polymerase subunit omega

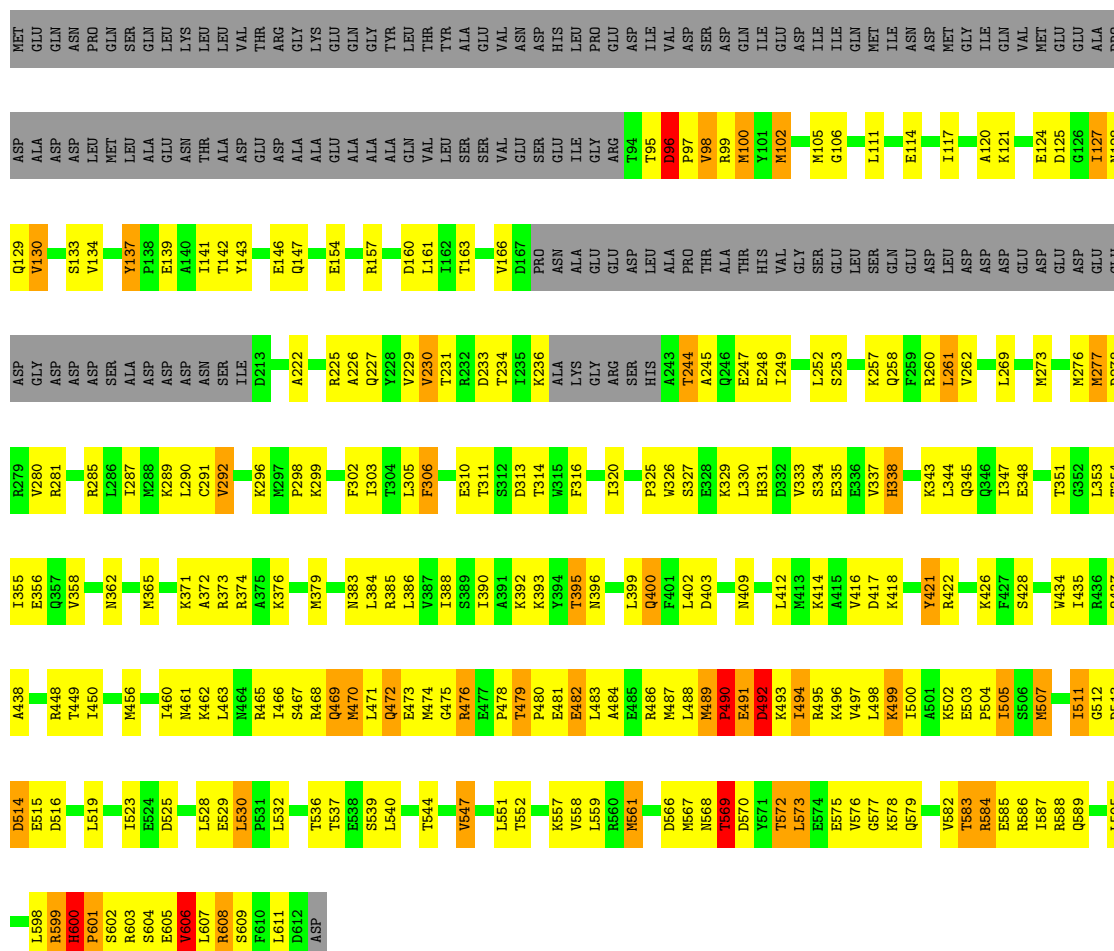
Chain E: 58% 34% 5%



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD



V558	E473	A391	K329	R260	GLU	ASP
L559	M474	K392	V333	L261	GLU	ALA
M560	G475	K393	V334	V262	ASP	ASP
R561	R476	Y394	P263	P264	GLY	ASP
R562	E477	T395	E335	K265	ASP	LEU
	P478	N396	E336	Q266	ASP	MET
I565	T479	R397	V337	F266	ASP	LEU
D566		G398	H338		SER	ALA
M567	E482	L399	R339	N271	ALA	ALA
N568	L483	A340	A341	S272	ALA	GLU
T569	A484	L402	L341	M273	ASP	ASN
D570	E485	D403	K342	R274	ASP	THR
Y571	R486	Q406	Q343	R275	ALA	ALA
T572	M487		L344	V276	ASP	ASP
L573	L488		Q345	M277	SER	GLU
E574	M489	N409	Q346		ILE	ASP
E575	P490	L412	I347	V280	D213	ALA
V576	E491	M413	E348	R281	L216	ALA
G577	D492	K414	E349	T282	A217	GLU
K578	K493	A415	E350	Q283	A218	ALA
Q579	I494	V416	T351	E284	R218	ALA
F580		D417	G352	R285	E219	ALA
D581	K499	D418	L353	L286	K220	ALA
V582	I500	K418	T354	L287	F221	GLN
T583		F419	I355	M288	A222	VAL
R584	E503	E420	E356	K289	E223	LEU
E585	P504	Y421	Q357	L290		SER
R586	I505	R422	V358	C291	A226	SER
T587			K359	V292	Q227	VAL
R588	E508	Y430	D360	E293	Y228	GLU
Q589		A431	I361		V229	GLU
	I511		N362	M297	V230	ILE
K597	G512	W434	R363	P298	T231	GLY
L598	D513	I435	R364	K299	R232	ARG
R599	D514		N365		D233	T94
H600	E515	I443	S366	F302	T234	T95
	D516		I367	I303	K235	D96
		R448	G368	T304	K236	P97
	L519	T449	E369	L305	ALA	V98
		I450	A370	F306	LYS	R99
	D525		K371		GLY	M100
R603	T526	P453	A372	E310	ARG	Y101
L607	T527	V454	R373	T311	SER	M102
R608		H455	R374	S312	HIS	M105
S609		M456	A375	D313	VAL	
F610	P531	I457	K376	T314	GLY	V108
L611	L532	E458	K377	W315	SER	
D612		T459	E378	F316	LEU	L111
D613	A535	I460	N379	N317	SER	T112
	T536		V380	A318	GLN	R113
		L463	E381	A319	GLU	E114
	L540	H464	A382	I320	ASP	G115
	T544	R465	N383	A321	LEU	E116
		I466	L384	M322	ASP	I117
	V547	S467	R385	N323	E254	D118
		R468	L386	K324	ASP	T119
	L551	Q469	V387	P325	GLU	A120
	T552	M470	I388	W326	ASP	K121
		L471	S389	Q257	GLU	
		Q472	I390	F259	ASP	E124

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	186.10Å 206.44Å 307.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.57 29.96 – 3.57	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.96-3.57) 92.1 (29.96-3.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.56Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.217 , 0.252 0.228 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (1.42%)	wwPDB-VP
Wilson B-factor (Å ²)	112.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55782	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% 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: MG, 4C6, ZN

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	1.03	0/2524	1.26	12/3421 (0.4%)
1	B	1.15	9/1697 (0.5%)	1.34	14/2300 (0.6%)
1	G	1.02	1/1777 (0.1%)	1.25	8/2408 (0.3%)
1	H	1.11	3/1681 (0.2%)	1.34	16/2278 (0.7%)
2	C	1.12	18/10739 (0.2%)	1.27	73/14489 (0.5%)
2	I	1.01	9/10735 (0.1%)	1.25	59/14484 (0.4%)
3	D	1.19	16/9188 (0.2%)	1.32	68/12404 (0.5%)
3	J	1.04	16/9128 (0.2%)	1.28	63/12322 (0.5%)
4	E	0.89	0/693	1.12	2/935 (0.2%)
4	K	1.45	4/629 (0.6%)	1.37	2/847 (0.2%)
5	F	1.10	5/3864 (0.1%)	1.27	22/5194 (0.4%)
5	L	1.08	9/3872 (0.2%)	1.21	10/5205 (0.2%)
All	All	1.09	90/56527 (0.2%)	1.28	349/76287 (0.5%)

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
2	C	0	3
2	I	0	4
3	D	0	2
3	J	0	1
5	F	0	1
All	All	0	11

The worst 5 of 90 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1296	ASP	CG-OD2	10.00	1.44	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	799	ARG	CB-CG	-9.11	1.25	1.52
1	H	14	VAL	CA-CB	9.02	1.65	1.54
2	C	1112	ILE	CA-CB	-8.57	1.43	1.54
2	I	975	ILE	CA-CB	8.24	1.63	1.54

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ALA	CA-C-N	-12.96	103.64	119.84
3	D	426	ALA	C-N-CA	-12.96	103.64	119.84
2	C	920	VAL	CA-C-N	11.63	131.74	119.76
2	C	920	VAL	C-N-CA	11.63	131.74	119.76
3	D	833	GLU	CA-C-N	11.32	131.08	120.21

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1264	GLN	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide

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	2490	0	2542	208	0
1	B	1677	0	1703	108	0
1	G	1755	0	1773	126	0
1	H	1662	0	1687	135	0
2	C	10570	0	10582	636	0
2	I	10566	0	10576	647	0
3	D	9050	0	9218	670	0
3	J	8990	0	9173	615	0
4	E	691	0	695	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	47	0
5	F	3813	0	3880	216	0
5	L	3821	0	3884	258	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	0	25	1	0
8	J	31	0	25	2	0
All	All	55782	0	56397	3392	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 30.

The worst 5 of 3392 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:G:190:ALA:HB2	1:G:200:LYS:HB2	1.29	1.14
1:A:45:ARG:HG2	1:B:38:THR:HB	1.31	1.12
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.30	1.08
2:I:1269:ARG:HD3	3:J:343:LEU:HD21	1.35	1.08
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.17	1.07

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	317/329 (96%)	243 (77%)	48 (15%)	26 (8%)	0 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/329 (65%)	193 (91%)	15 (7%)	5 (2%)	5	29
1	G	225/329 (68%)	195 (87%)	21 (9%)	9 (4%)	2	20
1	H	212/329 (64%)	193 (91%)	15 (7%)	4 (2%)	6	33
2	C	1338/1342 (100%)	1210 (90%)	111 (8%)	17 (1%)	9	39
2	I	1338/1342 (100%)	1207 (90%)	112 (8%)	19 (1%)	9	38
3	D	1157/1407 (82%)	1031 (89%)	101 (9%)	25 (2%)	5	30
3	J	1146/1407 (81%)	1032 (90%)	92 (8%)	22 (2%)	6	33
4	E	87/91 (96%)	81 (93%)	4 (5%)	2 (2%)	5	29
4	K	77/91 (85%)	73 (95%)	3 (4%)	1 (1%)	9	39
5	F	462/613 (75%)	424 (92%)	30 (6%)	8 (2%)	7	35
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	35
All	All	7035/8222 (86%)	6307 (90%)	582 (8%)	146 (2%)	5	31

5 of 146 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	107	ILE
1	A	114	ASP
1	A	136	GLU
1	A	195	ARG

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	278/286 (97%)	226 (81%)	52 (19%)	1	10
1	B	186/286 (65%)	162 (87%)	24 (13%)	4	22
1	G	193/286 (68%)	168 (87%)	25 (13%)	4	21
1	H	183/286 (64%)	163 (89%)	20 (11%)	6	27
2	C	1155/1157 (100%)	1018 (88%)	137 (12%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1026 (89%)	128 (11%)	6	27
3	D	964/1168 (82%)	847 (88%)	117 (12%)	5	24
3	J	962/1168 (82%)	851 (88%)	111 (12%)	5	25
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	27
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	33
5	F	417/540 (77%)	368 (88%)	49 (12%)	5	25
5	L	418/540 (77%)	363 (87%)	55 (13%)	4	21
All	All	6049/7024 (86%)	5317 (88%)	732 (12%)	5	24

5 of 732 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	321	LEU
3	J	175	GLU
2	I	492	MET
2	I	320	ASP
2	I	979	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	1237	HIS
3	J	702	GLN
2	I	1314	GLN
3	J	450	HIS
3	J	861	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	4C6	D	2004	-	32,34,34	0.99	1 (3%)	42,51,51	1.84	2 (4%)
8	4C6	J	2004	-	32,34,34	0.72	0	42,51,51	1.04	3 (7%)

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
8	4C6	D	2004	-	-	4/15/45/45	0/4/4/4
8	4C6	J	2004	-	-	2/15/45/45	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C6	S-N	-4.41	1.60	1.64

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2004	4C6	C5-C2-S	11.11	135.50	127.23
8	J	2004	4C6	C7-C21-C	-3.00	85.26	88.05
8	J	2004	4C6	C7-C1-N	2.62	135.43	129.88
8	D	2004	4C6	C7-C1-N	2.08	134.28	129.88
8	J	2004	4C6	C1-C-C21	2.07	89.98	88.30

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

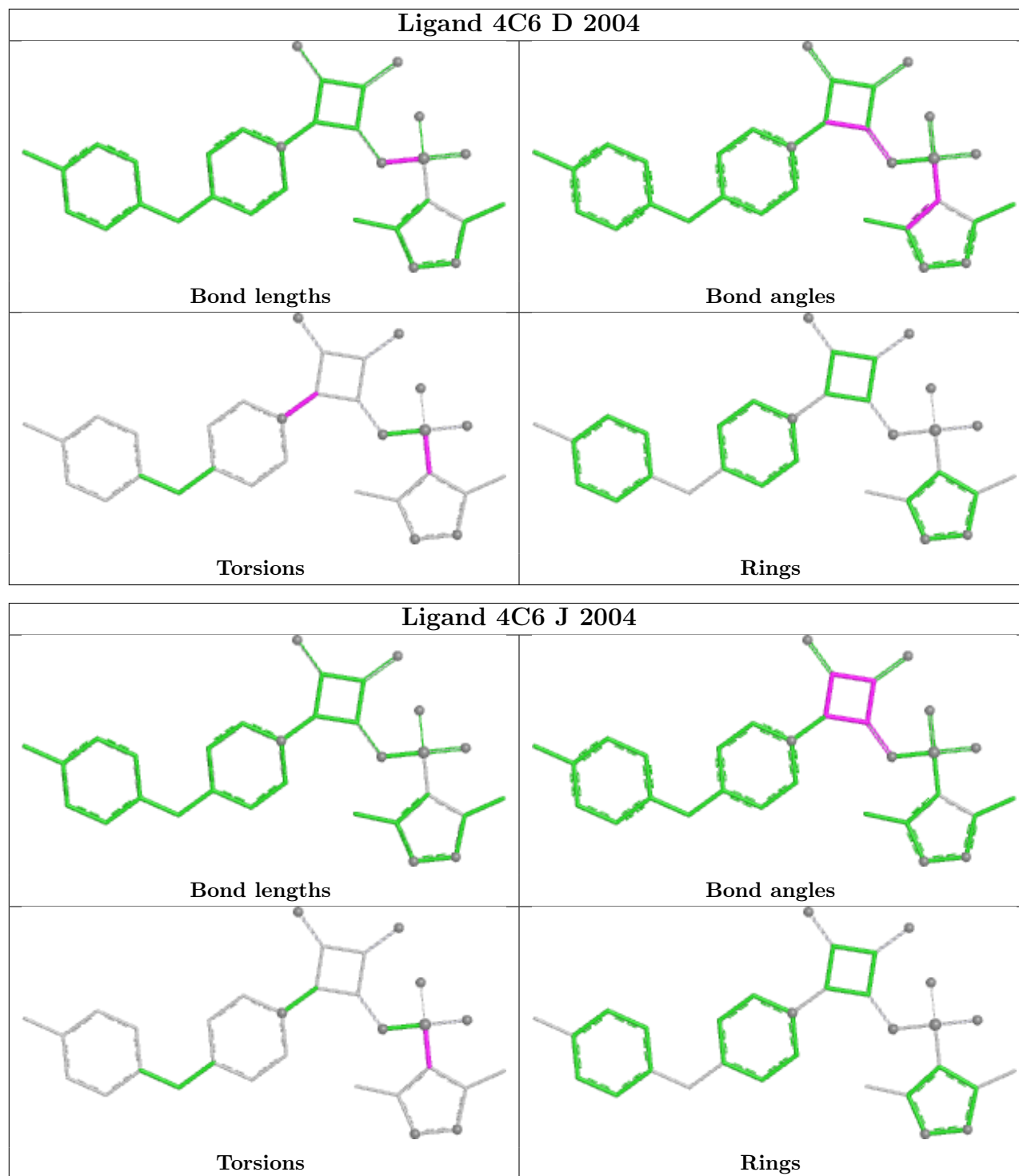
Mol	Chain	Res	Type	Atoms
8	D	2004	4C6	C3-C2-S-O2
8	D	2004	4C6	C3-C2-S-O3
8	D	2004	4C6	C5-C2-S-O3
8	J	2004	4C6	C3-C2-S-O3
8	J	2004	4C6	C3-C2-S-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C6	1	0
8	J	2004	4C6	2	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 ⓘ

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	319/329 (96%)	-0.77	0 100 100	105, 138, 176, 185	0
1	B	217/329 (65%)	-0.63	0 100 100	114, 172, 192, 198	0
1	G	227/329 (68%)	-0.69	0 100 100	138, 159, 175, 192	0
1	H	216/329 (65%)	-0.65	0 100 100	130, 174, 192, 201	0
2	C	1340/1342 (99%)	-0.73	0 100 100	88, 126, 202, 228	0
2	I	1340/1342 (99%)	-0.73	0 100 100	108, 154, 212, 314	0
3	D	1163/1407 (82%)	-0.74	0 100 100	90, 119, 164, 197	0
3	J	1152/1407 (81%)	-0.71	1 (0%) 92 85	103, 137, 181, 211	0
4	E	89/91 (97%)	-0.77	0 100 100	129, 159, 178, 184	0
4	K	79/91 (86%)	-0.58	0 100 100	186, 221, 249, 254	0
5	F	468/613 (76%)	-0.66	0 100 100	113, 159, 233, 249	0
5	L	469/613 (76%)	-0.71	0 100 100	127, 168, 244, 260	0
All	All	7079/8222 (86%)	-0.71	1 (0%) 100 100	88, 143, 205, 314	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1215	GLU	2.4

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

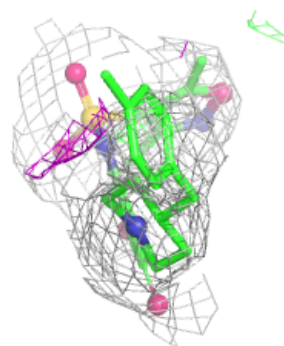
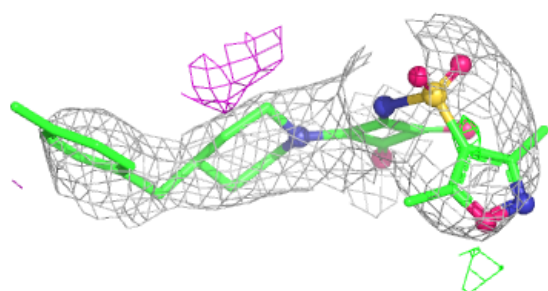
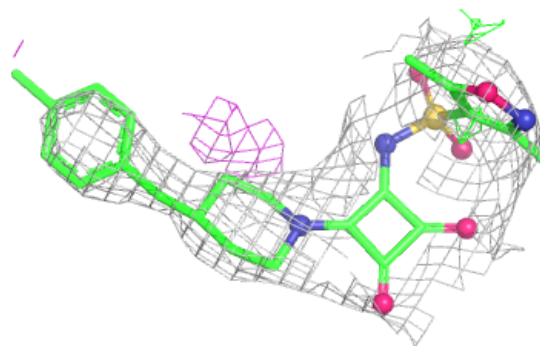
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	C	1401	1/1	0.57	0.21	127,127,127,127	0
6	MG	I	1401	1/1	0.63	0.20	127,127,127,127	0
6	MG	D	2001	1/1	0.80	0.15	127,127,127,127	0
6	MG	J	2001	1/1	0.85	0.15	127,127,127,127	0
8	4C6	J	2004	31/31	0.97	0.11	127,127,128,141	0
8	4C6	D	2004	31/31	0.98	0.16	127,127,127,127	0
7	ZN	J	2002	1/1	0.98	0.06	190,190,190,190	0
7	ZN	D	2002	1/1	0.99	0.10	164,164,164,164	0
7	ZN	D	2003	1/1	1.00	0.04	127,127,127,127	0
7	ZN	J	2003	1/1	1.00	0.03	127,127,127,127	0

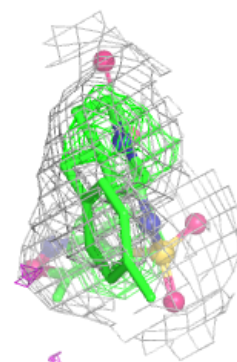
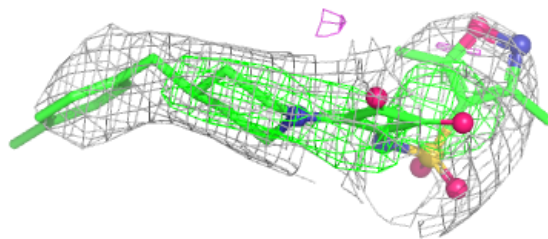
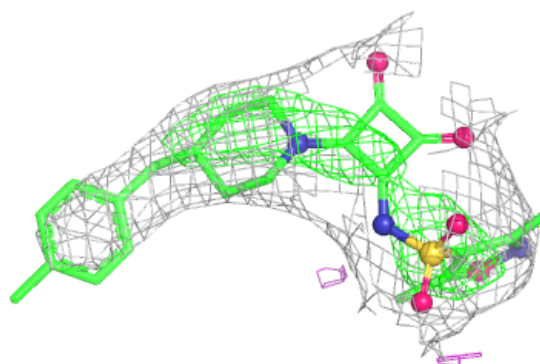
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4C6 J 2004:

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

**Electron density around 4C6 D 2004:**

$2mF_o-DF_c$ (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.