



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:45 PM UTC

PDB ID : 4YFN / pdb_00004yfn
Title : Escherichia coli RNA polymerase in complex with squaramide compound 14 (N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1-en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide)
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 : 3.82 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](#) ①) 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

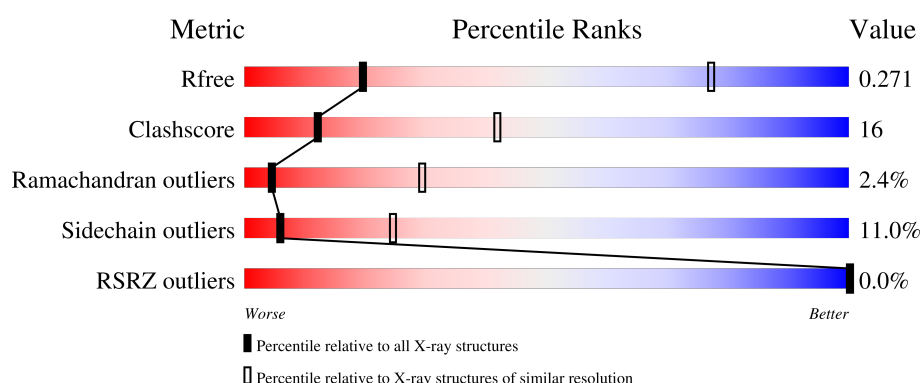
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 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.



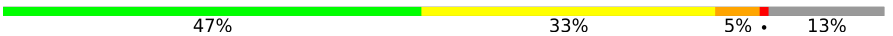
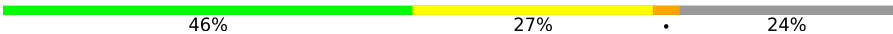
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	 62% 32% 6%
3	D	1407	 45% 30% 7% 17%
3	J	1407	 47% 28% 6% 18%
4	E	91	 73% 22% 5% 2%
4	K	91	 47% 33% 5% 13%
5	F	613	 46% 27% 5% 24%
5	L	613	 49% 22% 5% 23%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55638 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	235	Total	C	N	O	S	0	0	0
			1820	1132	323	358	7			
1	B	289	Total	C	N	O	S	0	0	0
			2234	1400	393	433	8			
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
			10560	6626	1837	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
			9029	5678	1613	1692	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8980	5648	1605	1681	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			

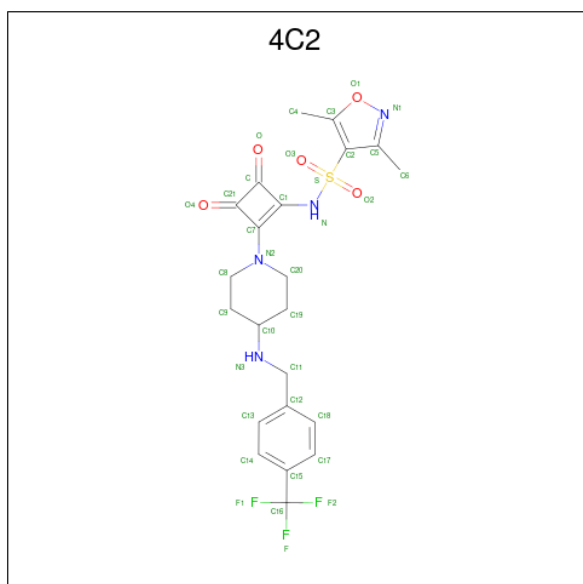
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	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 N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1-en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide (CCD ID: 4C2) (formula: C₂₂H₂₃F₃N₄O₅S).

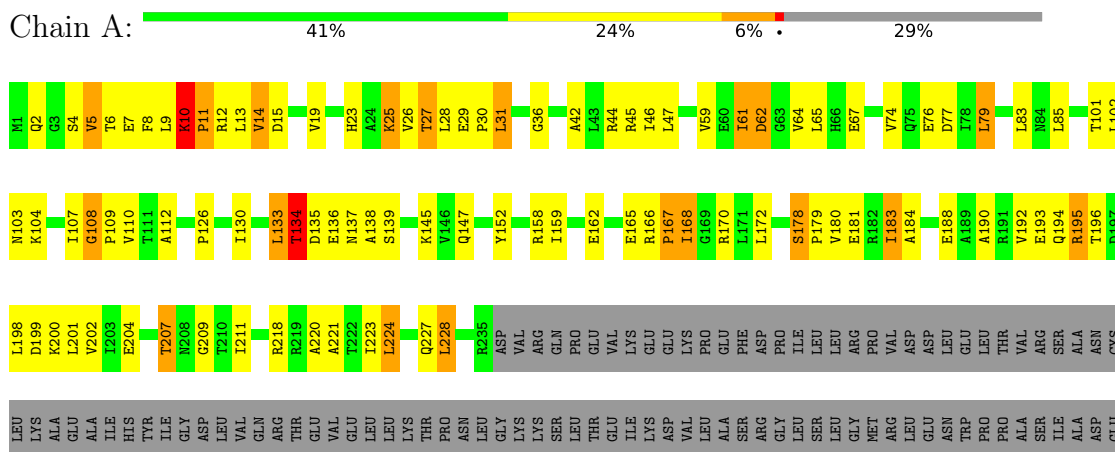


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		
8	J	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		

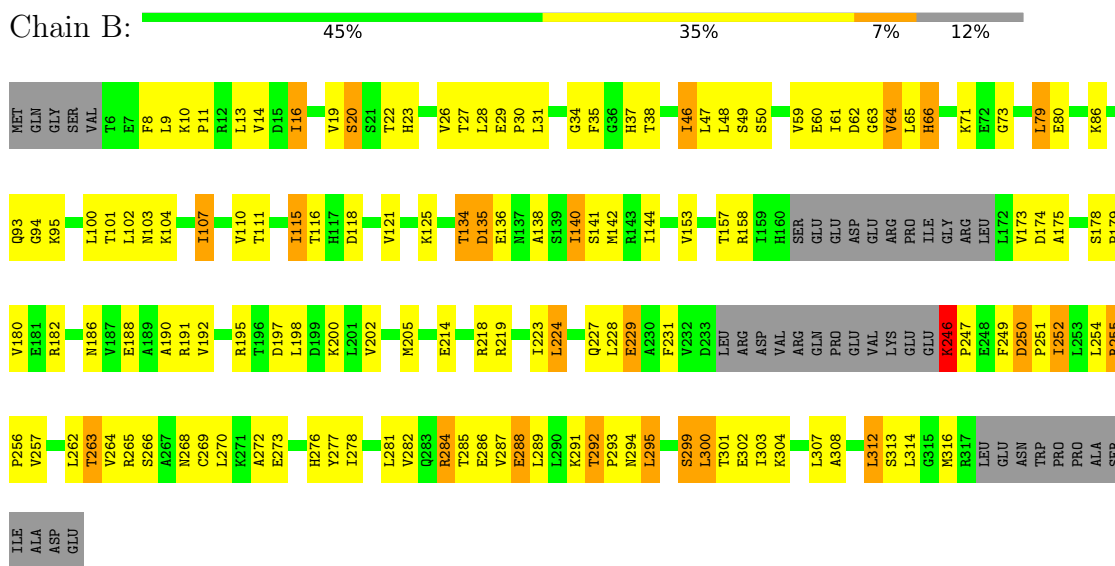
3 Residue-property plots

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

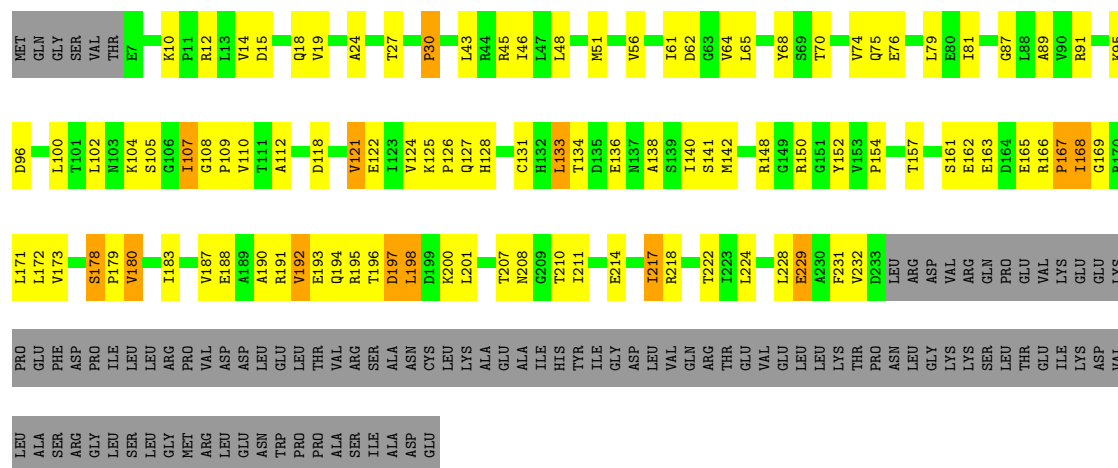


• Molecule 1: DNA-directed RNA polymerase subunit alpha

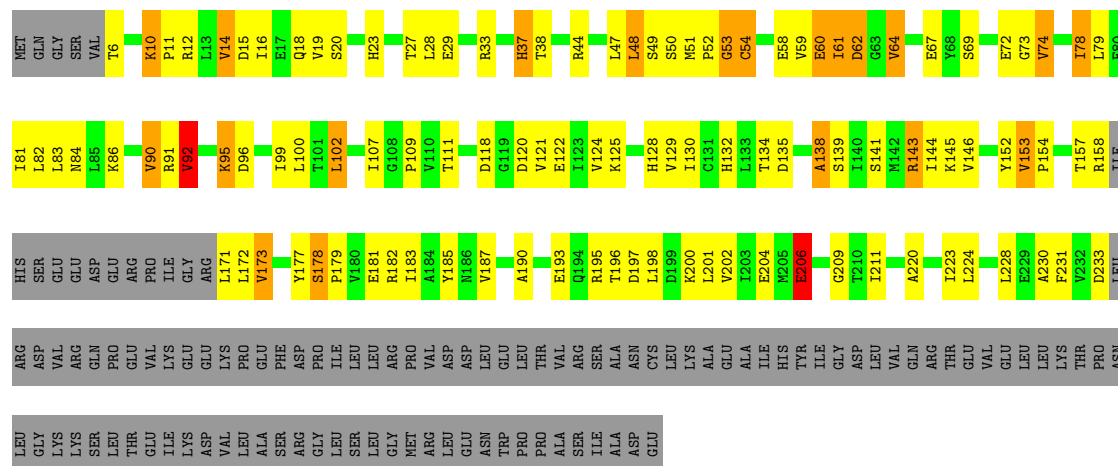


• Molecule 1: DNA-directed RNA polymerase subunit alpha

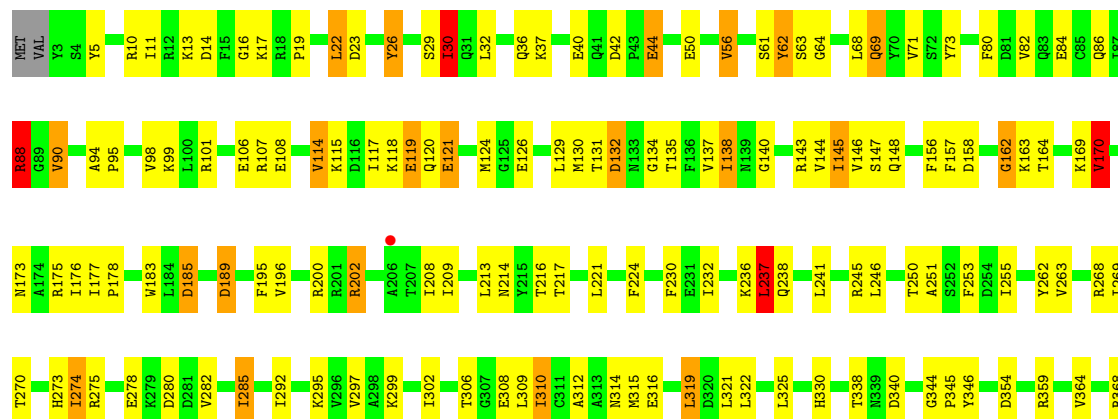


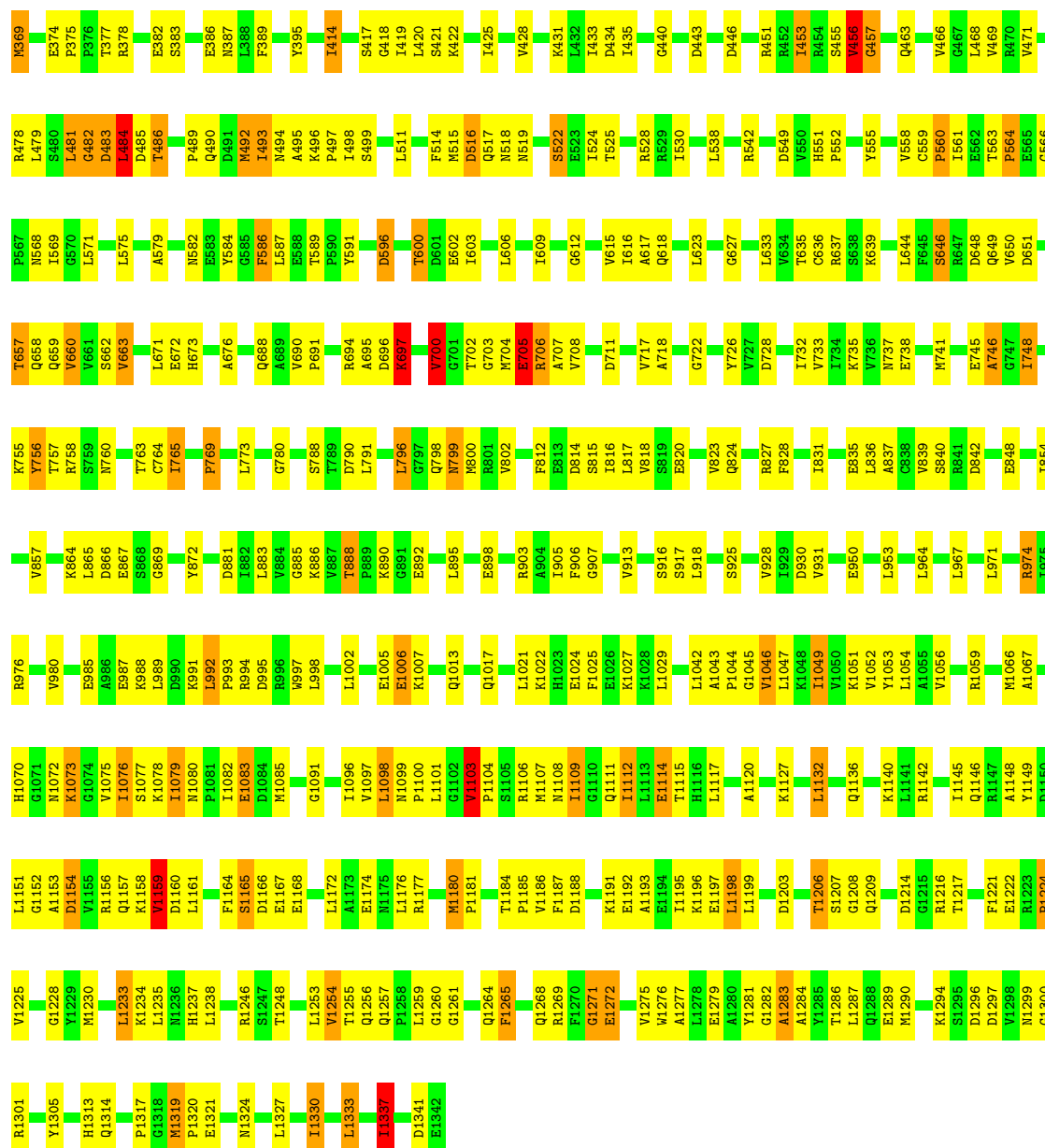


• Molecule 1: DNA-directed RNA polymerase subunit alpha



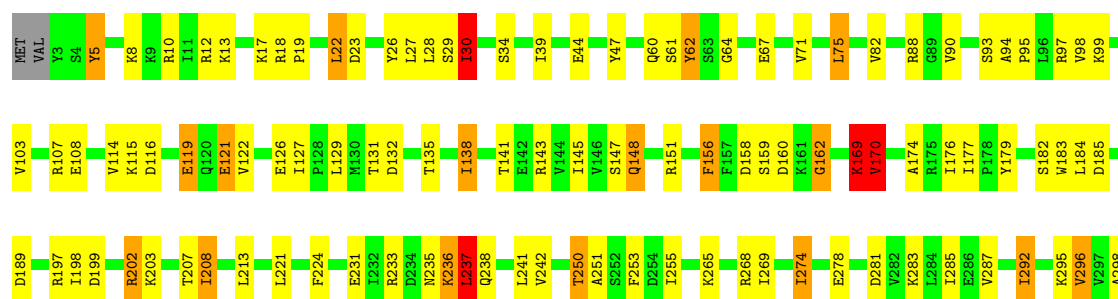
• Molecule 2: DNA-directed RNA polymerase subunit beta

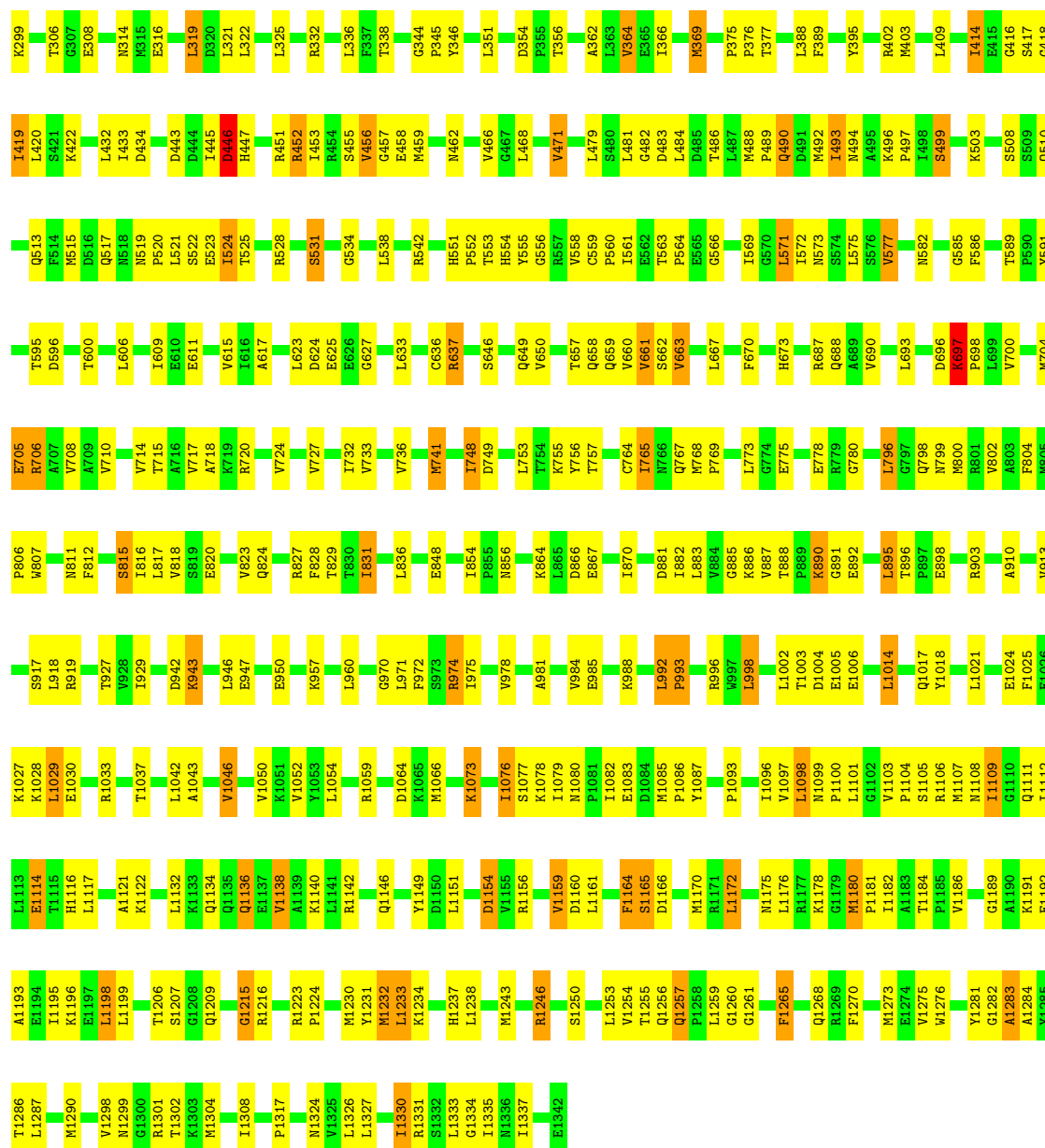




• Molecule 2: DNA-directed RNA polymerase subunit beta

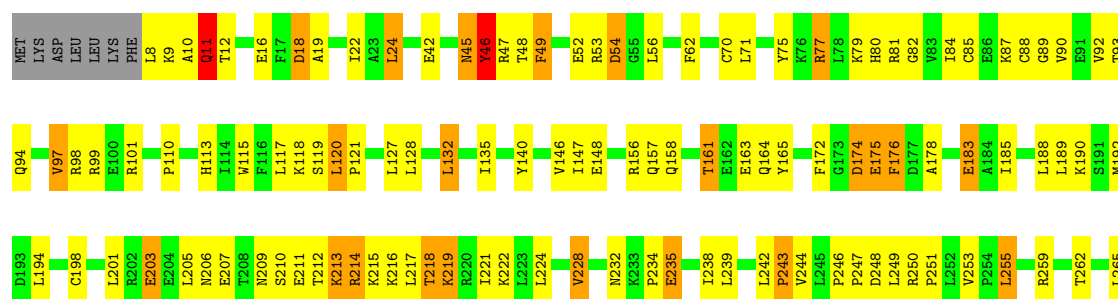
Chain I:





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

Chain D: 45% 30% 7% 17%



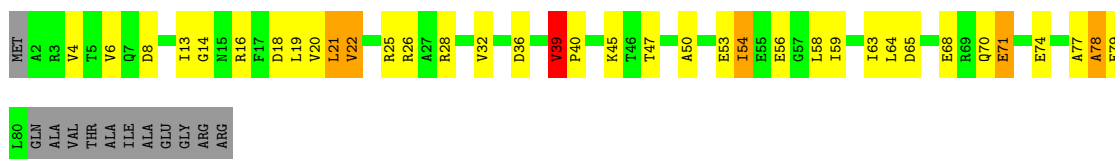


MET	LYS	ASP	LEU	LEU	LEU	PHE	LEU	LYS	GLN	THR	THR	GLU	F17	F17	A23	A25	S26	I30	K40	P41	T43	I44	N45	Y46	R47	T48	F49	E52	R53	D54	G55	L56	F57	F62	K66	E69	C70	L71	R77	L78	K79	H80	R81	G82	C85	E86					
K87	C88	G89	V90	E91	V92	T93	Q94	V97	R98	R101	W115	F116	L117	K118	S119	L120	R123	I124	L128	L132	R133	D134	I135	E136	R137	V138	L139	V146	I147	E148	L154	E155	R156	L160	T161	E162	Q164	Y165	L169	F172	G173	D174	E175	F176	Q186	A187					
L188	L189	M192	D193	Q196	E197	C198	V199	L201	R202	E203	E204	L205	N206	E207	T208	N209	S210	E211	K212	R214	K215	K216	L217	K219	R220	I221	K222	L223	L224	E225	V228	N232	K233	P234	E235	M236	M237	I238	T239	T240	V241	L242	P243	V244	L245	P246	P247	D248	P251	L252	L255
R259	L265	L268	R275	E276	R278	L279	L285	P288	D289	I290	I291	N294	E295	M298	L299	D304	A305	L306	R311	R312	T317	G318	S319	N320	L324	K325	M330	I331	Q335	GLY	ARG	PHE	R339	L342	L343	G344	V347	D348	Y349	S353	T356	Q448	L449	H450	P451	L452	V453	A459	D460		
F461	D462	G463	D464	Q465	L363	M466	L474	E475	Q477	L478	E479	A482	T487	N488	M489	L490	L491	S492	N495	G496	E497	P498	T499	I500	K501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548	
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
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K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548			
K549	V550	R551	Y555	E556	K557	D558	A559	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S319	V507	M513	T51																					

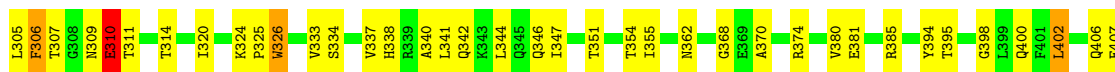
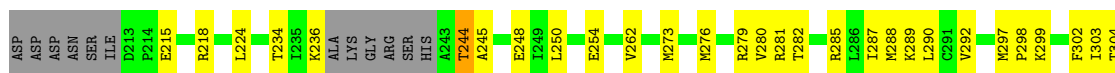
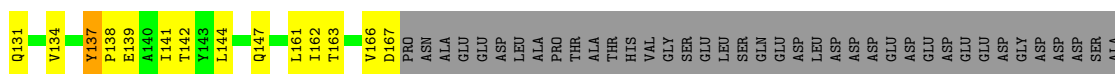
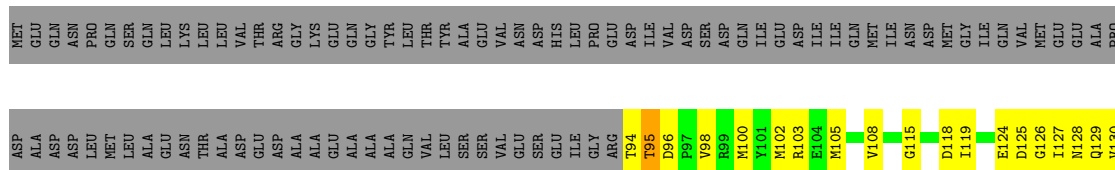
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 49% 22% 5% 23%

MET	GLU	GLN	ASN	PRO	GLN	SER	GLN	LEU	LYS	LEU	VAL	THR	ARG	GLY	LYS	GLU	GLN	GLY	TYR	LEU	THR	THR	TYR	ALA	GLU	VAL	ASN	ASP	HIS	LEU	PRO	GLU	ASP	ILE	VAL	ASP	SER	ASP	GLN	ILE	GLU	ILE	ILE	ASN	ASN	MET	GLY	ILE	GLN	VAL	MET	GLU	ALA	PRO					
ASP	ALA	ASP	ASP	LEU	MET	LEU	ALA	GLU	ASN	THR	ALA	ASP	GLU	ASP	ALA	ALA	ALA	GLU	GLU	ALA	GLN	VAL	LEU	LEU	SER	SER	GLU	VAL	ASN	ASP	HIS	LEU	GLY	ARG	T94	T95	D96	ASP	P97	V98	ASP	M102	ASP	M105	V108	E109	L110	R113	E114	I117	K121	E124	ASP	V130	ASP	V134	ASP		
Y137	P138	E139				T142	L144	L145	E146	Q147		V151			F165	V166	D167	PRO	ASN	GLU	ALA	ALA	THR	THR	THR	THR	THR	HIS	VAL	GLY	SER	GLY	ARG	LEU	GLN	SER	GLN	ASP	ASP	GLU	ASP	ASP	GLY	ASP	ASP	ASP	ASP	SER	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP			
ILE	D213		E219		L224			V229	V230	T231	R232	D233	T234	I235	K236	ALA	LYS	GLY	ARG	SER	HIS	A243	T244	A245	E248	K251	V255	R260	L269	V270	M273	R274	V275	M276	M277	V280	E284	K289	L290	C291	V292	C295	K296	M297	P298	K299		T304	L305	F306									
E310	T311			T314	V315	F316		K324	P325	W326		V333	S334		V337	L341	Q342	K343		E348		T351	G352	L353	D360	I361	N362	M365	S366	I367		K379	V380	E381	A382	N383	L384	R385	L386	V387	I388	K392		T395	Q400	F401	L402	Q406		L412		I435	R436						
Q437	D445			R448	T449	I450	R451	I452	P453	V454	H455	H456	I457		T466	S467	R468	Q469	M470	L471		M474	G475	R476	E477	P478	T479	P480	E481	E482	L483	A484	E485	R486	M487	L488	M489	P490	E491	D492	K493	I494	R495	K496	V497	L498	K499	I500		E503	P504	I505	S506	M507	E508	T509	P510	I511	G512
D513	T526	L530	T536	S539	L540	V547	L551	E555	V558	L559	R560	M561	D566	M567	R568	T569	D570	Y571	T572	L573	G577	D581	V582	T583	R584	I587	R588	A594	L598	R599	H600	P601	S602	R603	S604	R608	D612	D613																					

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	191.25Å 206.57Å 312.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.82 29.96 – 3.82	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.96-3.82) 77.7 (29.96-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.270 0.229 , 0.271	Depositor DCC
R_{free} test set	2003 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	136.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 123.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55638	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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, 4C2, 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	1.05	5/1842 (0.3%)	1.34	12/2495 (0.5%)
1	B	1.08	6/2260 (0.3%)	1.28	14/3059 (0.5%)
1	G	1.16	6/1777 (0.3%)	1.27	9/2408 (0.4%)
1	H	1.46	20/1681 (1.2%)	1.45	16/2278 (0.7%)
2	C	1.11	22/10739 (0.2%)	1.26	59/14489 (0.4%)
2	I	1.01	14/10729 (0.1%)	1.23	44/14477 (0.3%)
3	D	1.16	27/9167 (0.3%)	1.29	53/12380 (0.4%)
3	J	1.08	18/9118 (0.2%)	1.28	48/12312 (0.4%)
4	E	0.93	0/693	1.13	0/935
4	K	1.66	6/629 (1.0%)	1.57	8/847 (0.9%)
5	F	1.23	22/3864 (0.6%)	1.32	13/5194 (0.3%)
5	L	1.19	16/3872 (0.4%)	1.32	16/5205 (0.3%)
All	All	1.13	162/56371 (0.3%)	1.28	292/76079 (0.4%)

The worst 5 of 162 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	307	THR	CA-CB	10.09	1.65	1.53
1	H	111	THR	CA-CB	9.80	1.68	1.53
5	F	337	VAL	CA-CB	9.47	1.67	1.54
3	J	1190	ILE	CA-CB	9.01	1.61	1.54
2	C	90	VAL	CA-CB	-8.97	1.42	1.54

The worst 5 of 292 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ALA	CA-C-N	-14.60	103.63	120.13
3	D	426	ALA	C-N-CA	-14.60	103.63	120.13
3	J	17	PHE	N-CA-C	9.82	123.01	110.24
2	C	561	ILE	N-CA-C	9.75	119.80	111.90
1	B	250	ASP	CA-C-N	9.54	129.25	118.85

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	1820	0	1850	63	0
1	B	2234	0	2291	91	0
1	G	1755	0	1773	64	0
1	H	1662	0	1687	83	0
2	C	10570	0	10582	337	0
2	I	10560	0	10565	308	0
3	D	9029	0	9175	340	0
3	J	8980	0	9148	345	0
4	E	691	0	695	8	0
4	K	627	0	634	20	0
5	F	3813	0	3880	107	0
5	L	3821	0	3884	102	0
6	D	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	35	0	23	1	0
8	J	35	0	23	1	0
All	All	55638	0	56210	1746	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 16.

The worst 5 of 1746 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:255:ARG:HH11	1:B:255:ARG:HG3	1.24	1.03
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.39	1.01
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.46	0.94
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.48	0.93
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.53	0.91

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	233/329 (71%)	211 (91%)	16 (7%)	6 (3%)	4	28
1	B	283/329 (86%)	247 (87%)	28 (10%)	8 (3%)	4	27
1	G	225/329 (68%)	205 (91%)	15 (7%)	5 (2%)	5	30
1	H	212/329 (64%)	196 (92%)	14 (7%)	2 (1%)	14	46
2	C	1338/1342 (100%)	1194 (89%)	112 (8%)	32 (2%)	4	29
2	I	1338/1342 (100%)	1185 (89%)	122 (9%)	31 (2%)	5	30
3	D	1157/1407 (82%)	1036 (90%)	91 (8%)	30 (3%)	4	28
3	J	1146/1407 (81%)	1030 (90%)	85 (7%)	31 (3%)	4	27
4	E	87/91 (96%)	77 (88%)	6 (7%)	4 (5%)	2	19
4	K	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	9	39
5	F	462/613 (75%)	419 (91%)	34 (7%)	9 (2%)	6	33
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	34
All	All	7021/8222 (85%)	6294 (90%)	560 (8%)	167 (2%)	4	29

5 of 167 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	196	THR
1	B	13	LEU
1	B	50	SER
1	B	135	ASP

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	202/286 (71%)	175 (87%)	27 (13%)	4	19
1	B	248/286 (87%)	214 (86%)	34 (14%)	3	18
1	G	193/286 (68%)	177 (92%)	16 (8%)	10	34
1	H	183/286 (64%)	171 (93%)	12 (7%)	15	41
2	C	1155/1157 (100%)	1031 (89%)	124 (11%)	6	25
2	I	1153/1157 (100%)	1039 (90%)	114 (10%)	7	29
3	D	959/1168 (82%)	833 (87%)	126 (13%)	4	20
3	J	959/1168 (82%)	837 (87%)	122 (13%)	4	21
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	21
4	K	67/75 (89%)	56 (84%)	11 (16%)	2	14
5	F	417/540 (77%)	386 (93%)	31 (7%)	13	38
5	L	418/540 (77%)	383 (92%)	35 (8%)	10	34
All	All	6026/7024 (86%)	5365 (89%)	661 (11%)	6	24

5 of 661 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	1002	LEU
3	J	764	ARG
2	I	1140	LYS
2	I	992	LEU
3	J	244	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	472	GLN
3	J	1279	GLN
2	I	494	ASN
3	J	1268	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	L	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 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	4C2	D	2004	-	36,38,38	1.09	4 (11%)	49,58,58	1.59	8 (16%)
8	4C2	J	2004	-	36,38,38	0.43	0	49,58,58	1.72	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
8	4C2	D	2004	-	-	6/22/52/52	0/4/4/4
8	4C2	J	2004	-	-	3/22/52/52	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C2	C1-N	3.87	1.46	1.42
8	D	2004	4C2	C7-N2	-2.92	1.25	1.36
8	D	2004	4C2	O-C	-2.53	1.17	1.23
8	D	2004	4C2	C1-C7	-2.45	1.37	1.41

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C2	C5-C2-S	7.40	132.74	127.23
8	J	2004	4C2	C11-N3-C10	-6.28	103.43	113.84
8	J	2004	4C2	C19-C10-N3	-4.93	85.95	110.56
8	D	2004	4C2	C19-C10-N3	-4.88	86.20	110.56
8	D	2004	4C2	C1-C-C21	-4.71	84.47	88.30

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	2004	4C2	C3-C2-S-O2
8	D	2004	4C2	C3-C2-S-O3
8	D	2004	4C2	C9-C10-N3-C11
8	J	2004	4C2	C9-C10-N3-C11
8	D	2004	4C2	C5-C2-S-O2

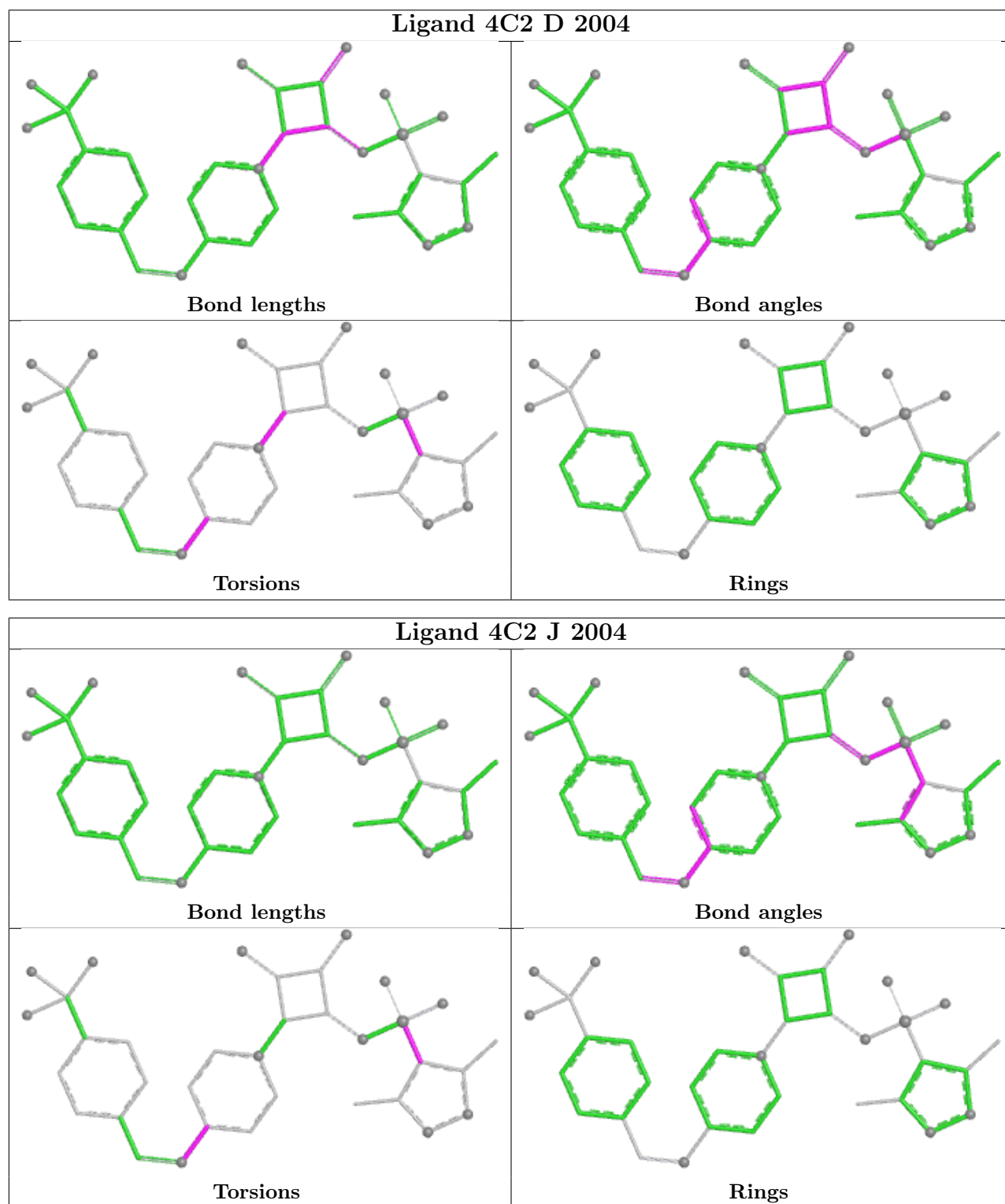
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C2	1	0
8	J	2004	4C2	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 ⓘ

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 [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	235/329 (71%)	-0.65	0 100 100	140, 166, 193, 222	0
1	B	289/329 (87%)	-0.65	0 100 100	146, 203, 247, 259	0
1	G	227/329 (68%)	-0.68	0 100 100	189, 214, 238, 246	0
1	H	216/329 (65%)	-0.49	0 100 100	201, 246, 255, 259	0
2	C	1340/1342 (99%)	-0.67	1 (0%) 92 87	115, 159, 222, 268	0
2	I	1340/1342 (99%)	-0.69	0 100 100	153, 185, 240, 340	0
3	D	1163/1407 (82%)	-0.64	0 100 100	121, 156, 213, 257	0
3	J	1152/1407 (81%)	-0.60	1 (0%) 92 87	151, 192, 247, 273	0
4	E	89/91 (97%)	-0.66	0 100 100	174, 192, 209, 216	0
4	K	79/91 (86%)	-0.52	0 100 100	262, 289, 297, 302	0
5	F	468/613 (76%)	-0.54	0 100 100	150, 211, 305, 326	0
5	L	469/613 (76%)	-0.61	0 100 100	163, 215, 294, 309	0
All	All	7067/8222 (85%)	-0.64	2 (0%) 100 100	115, 183, 255, 340	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1175	LEU	2.5
2	C	206	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

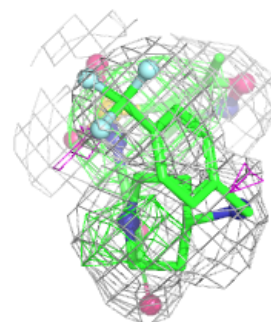
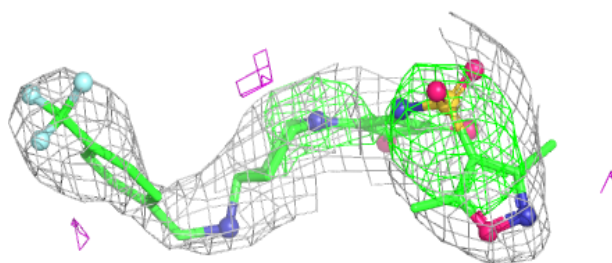
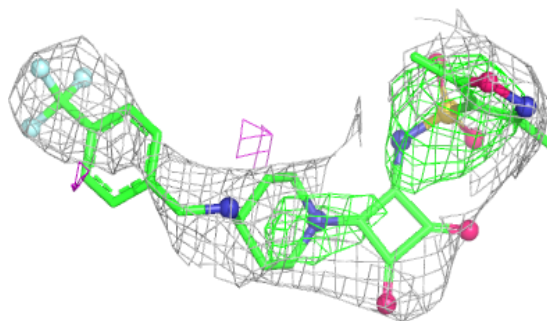
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	2001	1/1	0.93	0.08	166,166,166,166	0
6	MG	D	2001	1/1	0.97	0.04	166,166,166,166	0
8	4C2	D	2004	35/35	0.97	0.16	166,166,166,175	0
8	4C2	J	2004	35/35	0.98	0.08	166,166,171,175	0
7	ZN	J	2003	1/1	0.99	0.03	217,217,217,217	0
7	ZN	D	2002	1/1	0.99	0.05	166,166,166,166	0
7	ZN	J	2002	1/1	0.99	0.03	201,201,201,201	0
7	ZN	D	2003	1/1	1.00	0.07	166,166,166,166	0

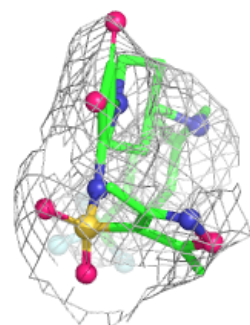
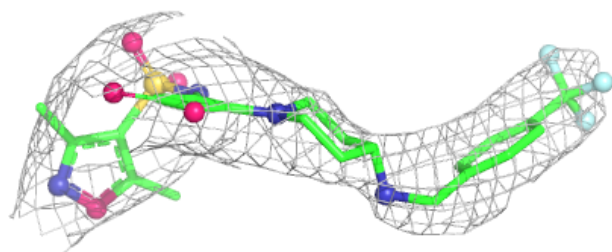
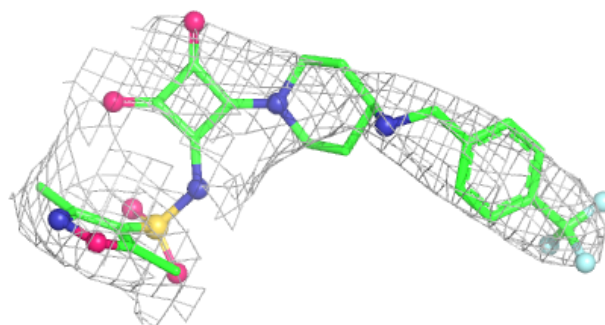
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4C2 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)

**Electron density around 4C2 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.