



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LLG
Title : Crystal Structure Analysis of the E.coli holoenzyme/Gp2 complex
Authors : Bae, B.; Darst, S.A.
Deposited on : 2013-07-09
Resolution : 3.79 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

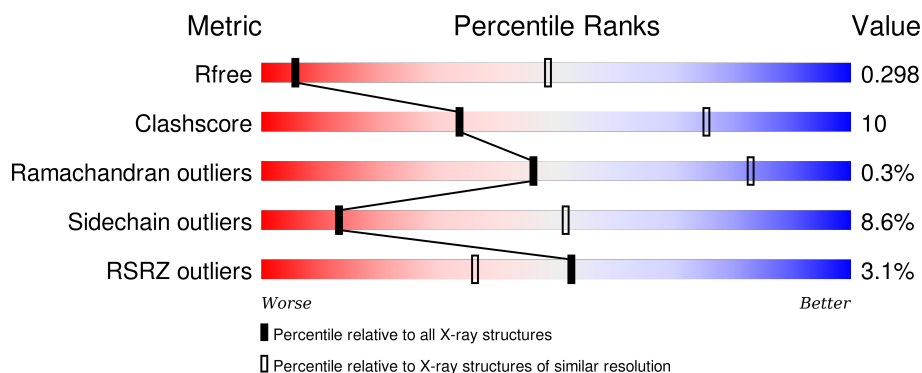
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.79 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	239	
1	B	239	
1	G	239	
1	H	239	
2	C	1342	

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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	
6	M	64	
6	N	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	ZN	D	1503	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 59147 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	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
A	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
A	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
A	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
A	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
B	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
B	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
B	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
B	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
B	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
G	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
G	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
G	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
G	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
G	239	GLN	-	EXPRESSION TAG	UNP C9QXI7
H	235	GLU	-	EXPRESSION TAG	UNP C9QXI7
H	236	VAL	-	EXPRESSION TAG	UNP C9QXI7
H	237	LEU	-	EXPRESSION TAG	UNP C9QXI7
H	238	PHE	-	EXPRESSION TAG	UNP C9QXI7
H	239	GLN	-	EXPRESSION TAG	UNP C9QXI7

- 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	1345	Total	C	N	O	S	0	0	0
			10447	6560	1864	1974	49			
3	J	1325	Total	C	N	O	S	0	0	0
			10295	6470	1831	1945	49			

- 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	521	Total	C	N	O	S	0	0	0
			4161	2609	735	791	26			
5	L	519	Total	C	N	O	S	0	0	0
			4155	2605	733	791	26			

- Molecule 6 is a protein called Bacterial RNA polymerase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	50	Total	C	N	O	S	0	0	0
			406	264	63	78	1			
6	N	48	Total	C	N	O	S	0	0	0
			389	253	60	75	1			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0

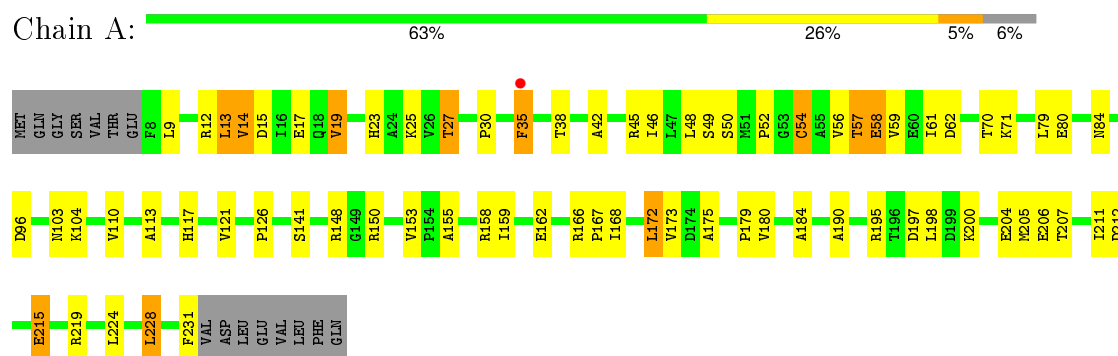
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

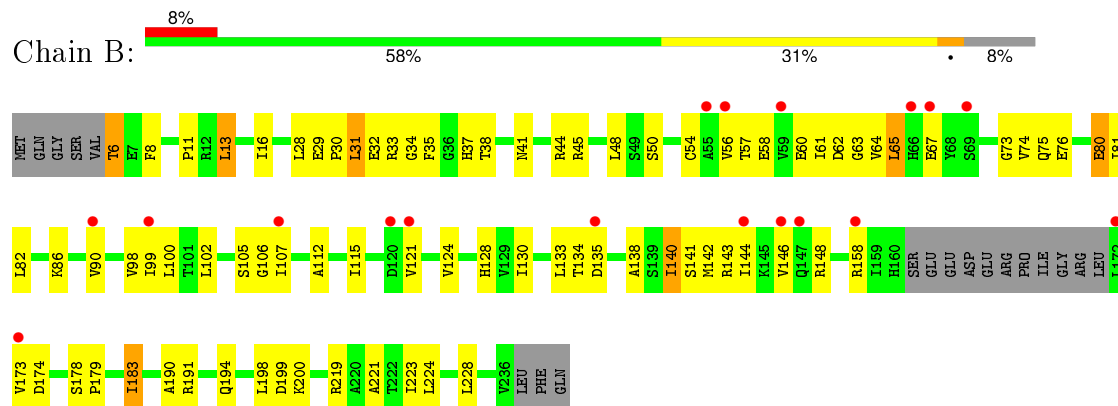
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

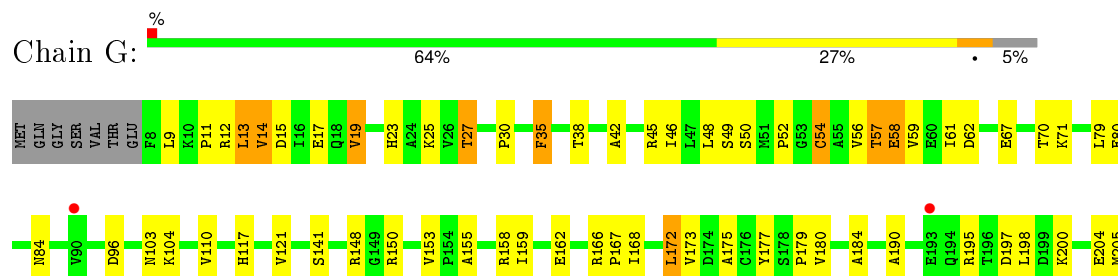
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

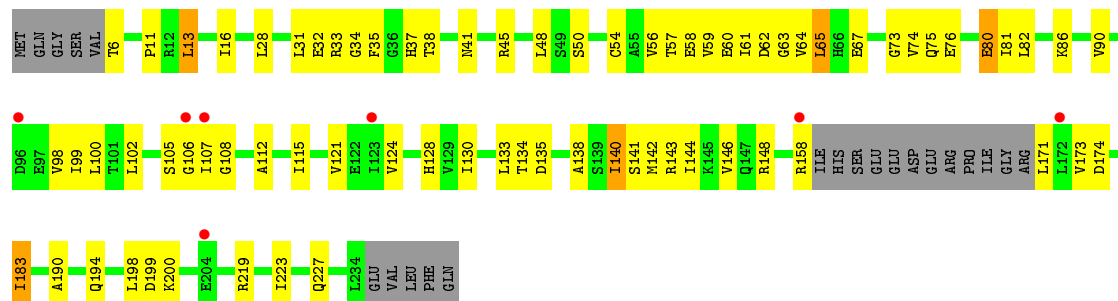


- Molecule 1: DNA-directed RNA polymerase subunit alpha

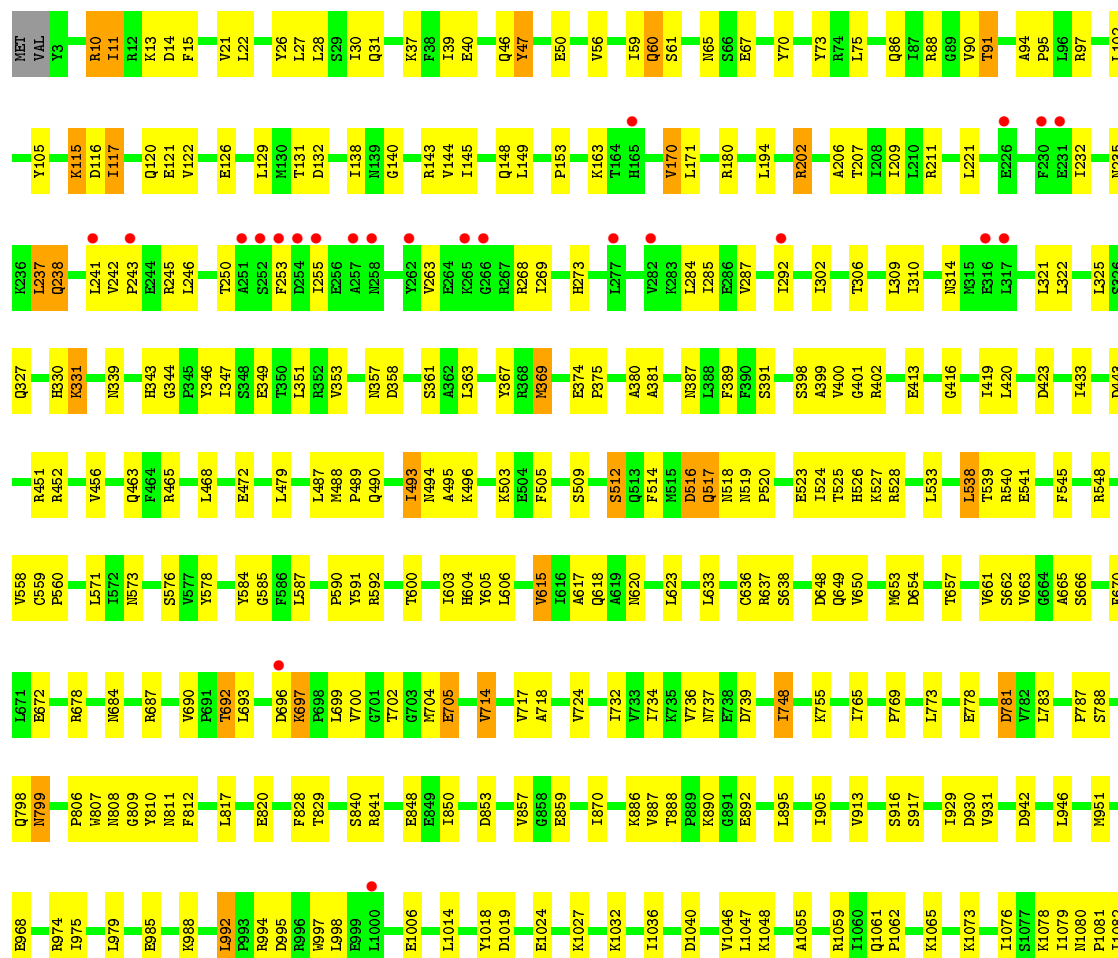


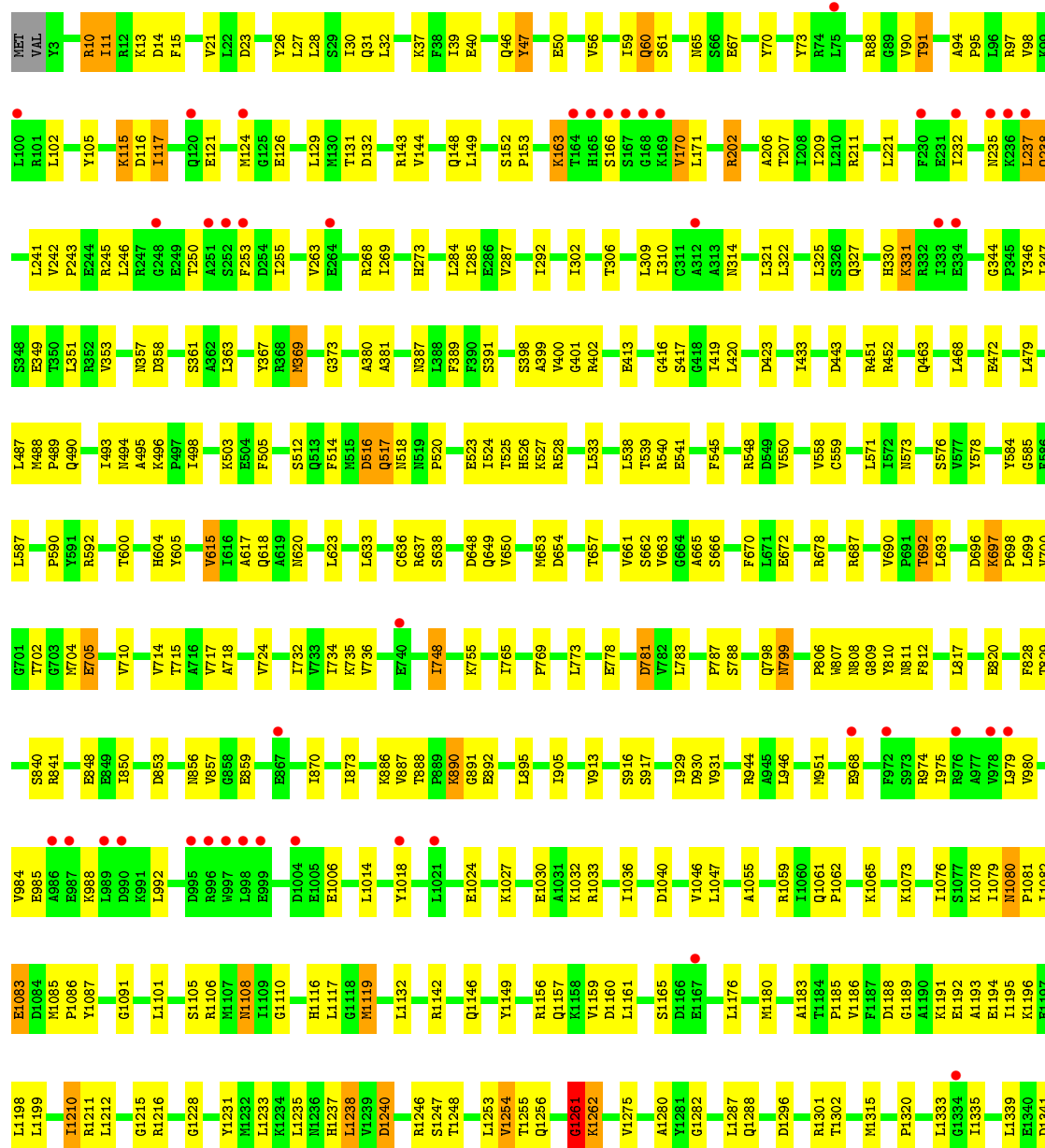


• Molecule 1: DNA-directed RNA polymerase subunit alpha

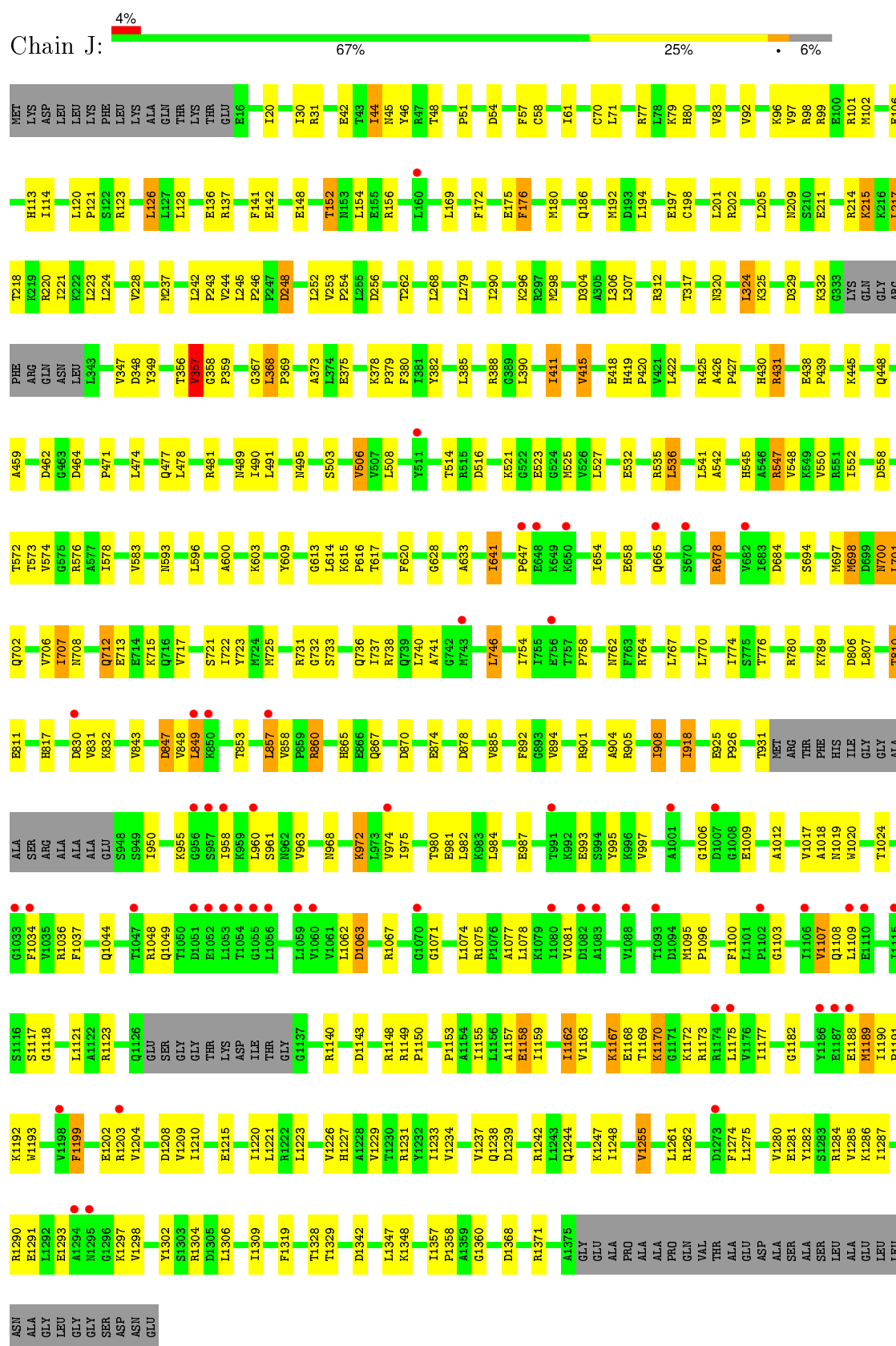


• Molecule 2: DNA-directed RNA polymerase subunit beta





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



- Molecule 4: DNA-directed RNA polymerase subunit omega

MEET A2 R3 Q7 T13 T14 R15 R16 F17 D18 R28 K35 D36 V39 D44 K45 T46 T47 V48 L58 I59 L64 R69 Q70 E71 Q72 Q73 E74 R90 ARG

- Chain K: 

- Chain F: 

Met	GLU	GLU	GLU	ASU	PRO	Q6	L9	K10	V13	T14	R15	Q19	Y21	L22	T23	P32	L35	V36	D39	Q40	I41	I44	I45	Q46	M47	I49	M51	G52	I53	Q54	V55	M56	GLU	GLU	ALA	ALA	PRO	ASP	ASP	ASP	ASP	LEU	LEU	ALA	GLU	ASU	THR	ALA	ALA	ASP	ASP	GLU
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ALA	ALA	GLU	ALA	ALA	ALA	GLN	VAL	LEU	SER	SER	VAL	GLU	SER	GLU	ILE	G92	V98	M105	L111	E114	I119	R122	I127	V130	V134	Y137	P138	E139	Q147	Y146	D149	R150	V151	E154	L158	L161	I162	T163	G164	F165	V166	D167	PRO	ASN	ALA
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GLU	GLU	ASP	LEU	ALA	PRO	THR	THR	VAL	GLY	SER	SER	LEU	GLU	SER	GLN	GLU	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASN	SER	SER	ILE	D213	A217	F221	R225	Q227	Y228	V229	F232	E236	ALA	LYS	GLY
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[illegible]

I347	E348	L353	T354	I356	R364	M365	V380	E381	L384	R385	F401	L402	I405	L412	V416	Y421	I435	R436	Q437	R448	T449	I450	V454	R455	M456	I457	I460	M461	R465	M470	L471	Q472	E473	E482	L483	A484	E485	R486	M487	L488	E491	V493
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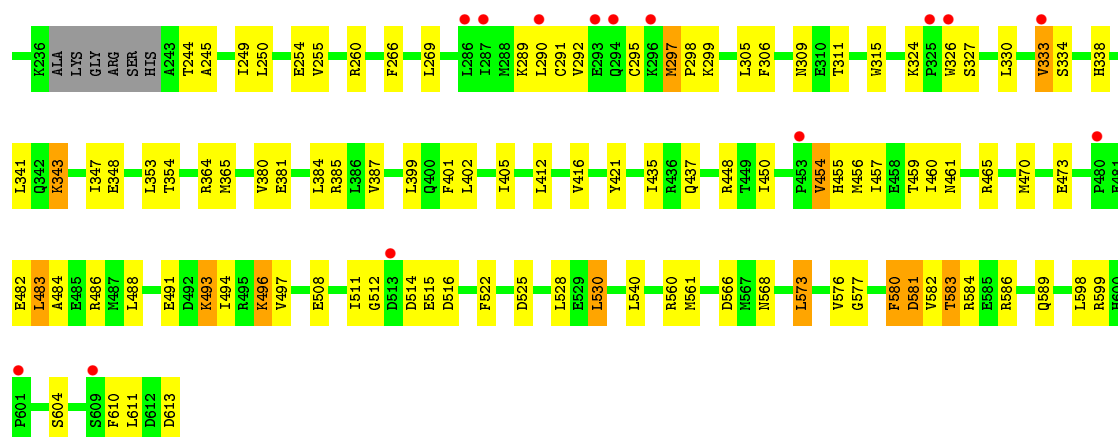
K493	L494	R495	K496	V497	E508	I511	G512	D513	D514	D516	F522	L528	E529	L530	P531	T536	R560	M561	R562	D566	M567	N568	L573	E574	E575	V576	G577	K578	K579	D581	F580	F581	V582	T583	R584	E585	R588	L598	R599	R603	G604	L611	D612
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- Chain L: 

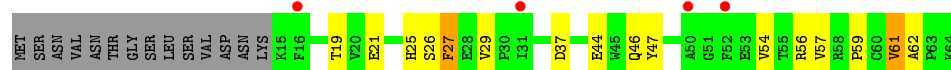
[illegible]

ALA	ALA	ALA	ALA	ALA	ALA	ALA	GLN	VAL	LEU	SER	SER	VAL	GLU	SER	GLU	ILE	GLY	ARG	T94	T95	T96	P96	P97	V98	R99	M105	L111	E114	I119	R122	G126	I127	V130	V134	Y137	P138	E139	Q147	I148	D149	R150	V151	E154	L158	I162	T163	C164	F165	F166	F167	F168	F169	F170	F171	F172	F173	F174	F175	F176	F177	F178	F179	F180	F181	F182	F183	F184	F185	F186	F187	F188	F189	F190	F191	F192	F193	F194	F195	F196	F197	F198	F199	F200	F201	F202	F203	F204	F205	F206	F207	F208	F209	F210	F211	F212	F213	F214	F215	F216	F217	F218	F219	F220	F221	F222	F223	F224	F225	F226	F227	F228	F229	F230	F231	F232	F233	F234	F235	F236	F237	F238	F239	F240	F241	F242	F243	F244	F245	F246	F247	F248	F249	F250	F251	F252	F253	F254	F255	F256	F257	F258	F259	F260	F261	F262	F263	F264	F265	F266	F267	F268	F269	F270	F271	F272	F273	F274	F275	F276	F277	F278	F279	F280	F281	F282	F283	F284	F285	F286	F287	F288	F289	F290	F291	F292	F293	F294	F295	F296	F297	F298	F299	F300	F301	F302	F303	F304	F305	F306	F307	F308	F309	F310	F311	F312	F313	F314	F315	F316	F317	F318	F319	F320	F321	F322	F323	F324	F325	F326	F327	F328	F329	F330	F331	F332	F333	F334	F335	F336	F337	F338	F339	F340	F341	F342	F343	F344	F345	F346	F347	F348	F349	F350	F351	F352	F353	F354	F355	F356	F357	F358	F359	F360	F361	F362	F363	F364	F365	F366	F367	F368	F369	F370	F371	F372	F373	F374	F375	F376	F377	F378	F379	F380	F381	F382	F383	F384	F385	F386	F387	F388	F389	F390	F391	F392	F393	F394	F395	F396	F397	F398	F399	F400	F401	F402	F403	F404	F405	F406	F407	F408	F409	F410	F411	F412	F413	F414	F415	F416	F417	F418	F419	F420	F421	F422	F423	F424	F425	F426	F427	F428	F429	F430	F431	F432	F433	F434	F435	F436	F437	F438	F439	F440	F441	F442	F443	F444	F445	F446	F447	F448	F449	F450	F451	F452	F453	F454	F455	F456	F457	F458	F459	F460	F461	F462	F463	F464	F465	F466	F467	F468	F469	F470	F471	F472	F473	F474	F475	F476	F477	F478	F479	F480	F481	F482	F483	F484	F485	F486	F487	F488	F489	F490	F491	F492	F493	F494	F495	F496	F497	F498	F499	F500	F501	F502	F503	F504	F505	F506	F507	F508	F509	F510	F511	F512	F513	F514	F515	F516	F517	F518	F519	F520	F521	F522	F523	F524	F525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608	F609	F610	F611	F612	F613	F614	F615	F616	F617	F618	F619	F620	F621	F622	F623	F624	F625	F626	F627	F628	F629	F630	F631	F632
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V166
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ILE
D213
A217
F221
R225
A226
Q227
V228
V229
F232



- Molecule 6: Bacterial RNA polymerase inhibitor



- Molecule 6: Bacterial RNA polymerase inhibitor



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.51Å 205.04Å 308.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.21 – 3.79 45.21 – 3.79	Depositor EDS
% Data completeness (in resolution range)	98.1 (45.21-3.79) 98.2 (45.21-3.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 3.77Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.282 0.263 , 0.298	Depositor DCC
R_{free} test set	5813 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	126.7	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 26.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 115910 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	59147	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MG

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	0.23	0/1751	0.49	0/2373
1	B	0.23	0/1707	0.45	0/2314
1	G	0.22	0/1771	0.49	0/2401
1	H	0.22	0/1686	0.45	0/2285
2	C	0.26	2/10739 (0.0%)	0.45	2/14489 (0.0%)
2	I	0.26	2/10735 (0.0%)	0.45	2/14484 (0.0%)
3	D	0.24	1/10603 (0.0%)	0.45	1/14316 (0.0%)
3	J	0.24	1/10450 (0.0%)	0.44	1/14112 (0.0%)
4	E	0.23	0/693	0.50	0/935
4	K	0.22	0/629	0.49	0/847
5	F	0.26	0/4214	0.49	2/5673 (0.0%)
5	L	0.27	0/4208	0.49	2/5665 (0.0%)
6	M	0.31	0/419	0.50	0/572
6	N	0.33	0/401	0.54	0/549
All	All	0.25	6/60006 (0.0%)	0.46	10/81015 (0.0%)

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	1
2	I	0	1
4	E	0	1
4	K	0	1
5	L	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	31	GLN	CD-NE2	-8.70	1.11	1.32
2	I	31	GLN	CD-NE2	-8.41	1.11	1.32
2	I	31	GLN	CD-OE1	-7.96	1.06	1.24
2	C	31	GLN	CD-OE1	-7.79	1.06	1.24
3	D	477	GLN	CD-NE2	-6.25	1.17	1.32

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	19	GLN	C-N-CA	6.02	134.94	122.30
2	I	1261	GLY	N-CA-C	5.91	127.87	113.10
2	C	1261	GLY	N-CA-C	5.90	127.84	113.10
3	J	1182	GLY	N-CA-C	5.72	127.39	113.10
5	F	19	GLN	C-N-CA	5.71	134.30	122.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1261	GLY	Peptide
4	E	14	GLY	Peptide
2	I	1261	GLY	Peptide
4	K	14	GLY	Peptide
5	L	19	GLN	Peptide

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	1730	0	1756	48	0
1	B	1687	0	1700	49	0
1	G	1750	0	1764	48	0
1	H	1667	0	1689	41	0
2	C	10570	0	10582	232	0
2	I	10566	0	10576	217	0
3	D	10447	0	10671	249	0
3	J	10295	0	10510	229	0
4	E	691	0	695	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	17	0
5	F	4161	0	4171	81	0
5	L	4155	0	4168	85	0
6	M	406	0	383	10	0
6	N	389	0	363	13	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	59147	0	59662	1210	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 10.

The worst 5 of 1210 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)
3:D:1173:ARG:HE	3:D:1192:LYS:HG3	1.29	0.97
3:J:1173:ARG:HE	3:J:1192:LYS:HG3	1.28	0.97
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
3:J:1006:GLY:H	3:J:1009:GLU:HG3	1.41	0.85
3:J:418:GLU:HG3	4:K:45:LYS:H	1.41	0.83

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	222/239 (93%)	194 (87%)	26 (12%)	2 (1%)	21	68
1	B	216/239 (90%)	187 (87%)	29 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	226/239 (95%)	197 (87%)	26 (12%)	3 (1%)	15	61
1	H	213/239 (89%)	187 (88%)	26 (12%)	0	100	100
2	C	1338/1342 (100%)	1213 (91%)	121 (9%)	4 (0%)	46	83
2	I	1338/1342 (100%)	1210 (90%)	124 (9%)	4 (0%)	46	83
3	D	1339/1407 (95%)	1229 (92%)	108 (8%)	2 (0%)	56	90
3	J	1317/1407 (94%)	1217 (92%)	98 (7%)	2 (0%)	52	86
4	E	87/91 (96%)	74 (85%)	12 (14%)	1 (1%)	17	65
4	K	77/91 (85%)	68 (88%)	8 (10%)	1 (1%)	15	61
5	F	513/613 (84%)	471 (92%)	42 (8%)	0	100	100
5	L	511/613 (83%)	469 (92%)	41 (8%)	1 (0%)	52	86
6	M	48/64 (75%)	43 (90%)	4 (8%)	1 (2%)	9	53
6	N	46/64 (72%)	42 (91%)	3 (6%)	1 (2%)	8	52
All	All	7491/7990 (94%)	6801 (91%)	668 (9%)	22 (0%)	46	83

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	N	61	VAL
2	C	170	VAL
2	C	1262	LYS
2	I	170	VAL
2	I	1262	LYS

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	191/206 (93%)	175 (92%)	16 (8%)	14	52
1	B	184/206 (89%)	166 (90%)	18 (10%)	10	44
1	G	191/206 (93%)	175 (92%)	16 (8%)	14	52
1	H	183/206 (89%)	168 (92%)	15 (8%)	14	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1155/1157 (100%)	1059 (92%)	96 (8%)	14	52
2	I	1154/1157 (100%)	1061 (92%)	93 (8%)	15	54
3	D	1125/1168 (96%)	1030 (92%)	95 (8%)	14	52
3	J	1110/1168 (95%)	1017 (92%)	93 (8%)	14	52
4	E	72/75 (96%)	65 (90%)	7 (10%)	10	45
4	K	67/75 (89%)	59 (88%)	8 (12%)	6	35
5	F	444/540 (82%)	400 (90%)	44 (10%)	10	44
5	L	445/540 (82%)	400 (90%)	45 (10%)	9	43
6	M	43/56 (77%)	39 (91%)	4 (9%)	11	47
6	N	41/56 (73%)	37 (90%)	4 (10%)	10	44
All	All	6405/6816 (94%)	5851 (91%)	554 (9%)	13	51

5 of 554 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	244	THR
2	I	47	TYR
5	L	98	VAL
5	F	364	ARG
1	G	35	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	31	GLN
2	I	1061	GLN
3	J	680	ASN
3	D	736	GLN
3	J	477	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - 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, 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	224/239 (93%)	0.09	1 (0%) 93 87	45, 79, 110, 138	0
1	B	220/239 (92%)	0.26	18 (8%) 14 9	54, 96, 118, 134	0
1	G	228/239 (95%)	-0.02	2 (0%) 85 74	49, 82, 112, 136	0
1	H	217/239 (90%)	0.15	7 (3%) 51 35	58, 98, 119, 135	0
2	C	1340/1342 (99%)	0.03	23 (1%) 73 58	24, 72, 107, 132	0
2	I	1340/1342 (99%)	0.07	44 (3%) 50 34	29, 76, 113, 139	0
3	D	1345/1407 (95%)	0.13	42 (3%) 52 36	26, 67, 119, 138	0
3	J	1325/1407 (94%)	0.13	54 (4%) 41 27	27, 68, 114, 137	0
4	E	89/91 (97%)	-0.16	0 100 100	30, 69, 97, 111	0
4	K	79/91 (86%)	-0.08	2 (2%) 61 44	32, 71, 107, 119	0
5	F	521/613 (84%)	0.14	18 (3%) 48 32	35, 93, 119, 135	0
5	L	519/613 (84%)	0.15	19 (3%) 45 30	39, 93, 119, 138	0
6	M	50/64 (78%)	0.39	4 (8%) 15 9	71, 92, 116, 127	0
6	N	48/64 (75%)	0.56	3 (6%) 23 14	75, 96, 117, 125	0
All	All	7545/7990 (94%)	0.10	237 (3%) 52 36	24, 77, 116, 139	0

The worst 5 of 237 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	252	SER	8.7
3	J	1054	THR	8.0
5	F	167	ASP	7.0
3	J	1053	LEU	6.8
2	C	257	ALA	6.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
8	ZN	D	1503	1/1	0.96	0.43	3.78	278,278,278,278	0
8	ZN	J	1503	1/1	0.99	0.19	-0.70	57,57,57,57	0
8	ZN	D	1502	1/1	0.98	0.12	-0.90	103,103,103,103	0
8	ZN	J	1502	1/1	0.97	0.15	-1.00	168,168,168,168	0
7	MG	D	1501	1/1	0.84	0.62	-	51,51,51,51	0
7	MG	J	1501	1/1	0.90	0.71	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.