



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 10:35 PM UTC

PDB ID : 3K70 / pdb_00003k70
Title : Crystal structure of the complete initiation complex of RecBCD
Authors : Saikrishnan, K.; Wigley, D.B.
Deposited on : 2009-10-11
Resolution : 3.59 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
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

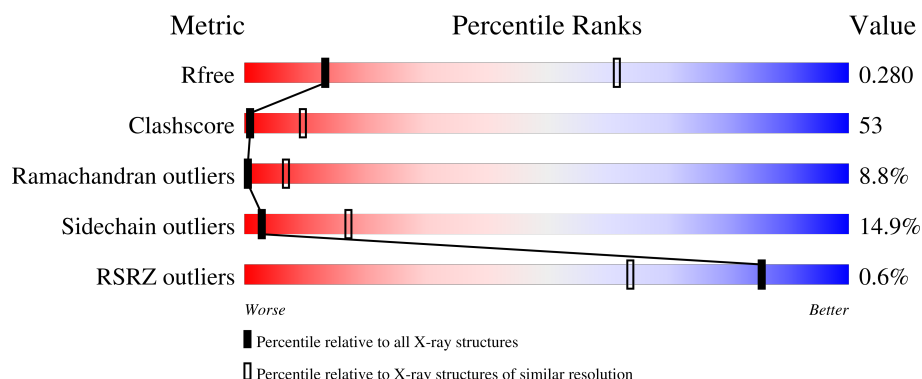
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	B	1180	
1	E	1180	
2	C	1122	
2	F	1122	
3	D	608	

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Mol	Chain	Length	Quality of chain
3	G	608	
4	X	51	
4	Y	51	

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
4	5IU	X	2	-	-	X	-
4	5IU	X	3	-	-	X	-
4	5IU	X	46	-	-	X	-
4	5IU	Y	2	-	-	X	-
4	5IU	Y	3	-	-	X	-
4	5IU	Y	46	-	-	X	-
4	5IU	Y	7	-	-	X	-
4	5IU	Y	9	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46932 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 Exodeoxyribonuclease V beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			
1	E	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			

- Molecule 2 is a protein called Exodeoxyribonuclease V gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			
2	F	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			

- Molecule 3 is a protein called Exodeoxyribonuclease V alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			
3	G	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			

- Molecule 4 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	X	46	Total	C	I	N	O	P	0	0	0
			935	442	9	164	276	44			
4	Y	46	Total	C	I	N	O	P	0	0	0
			935	442	9	164	276	44			

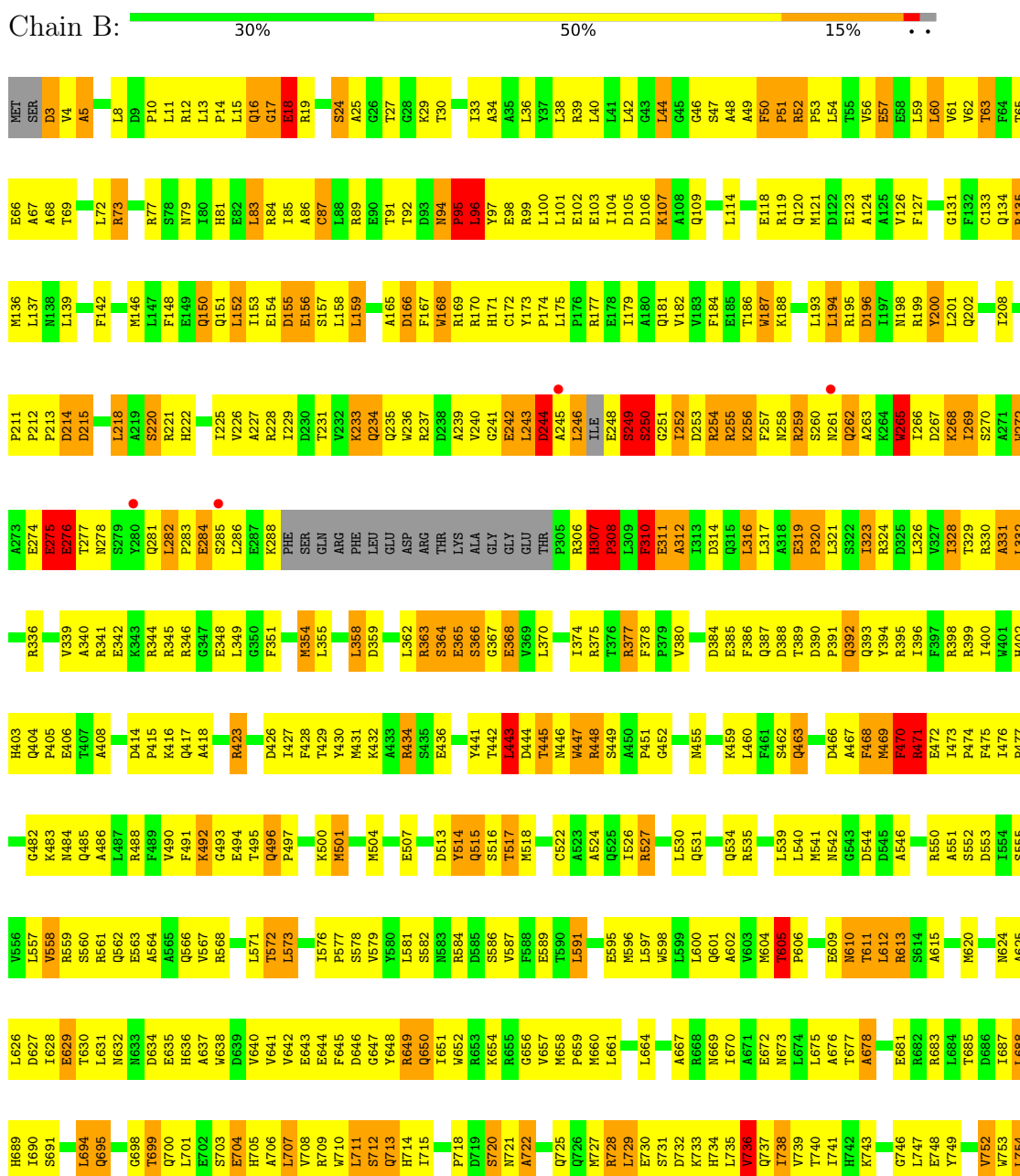
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

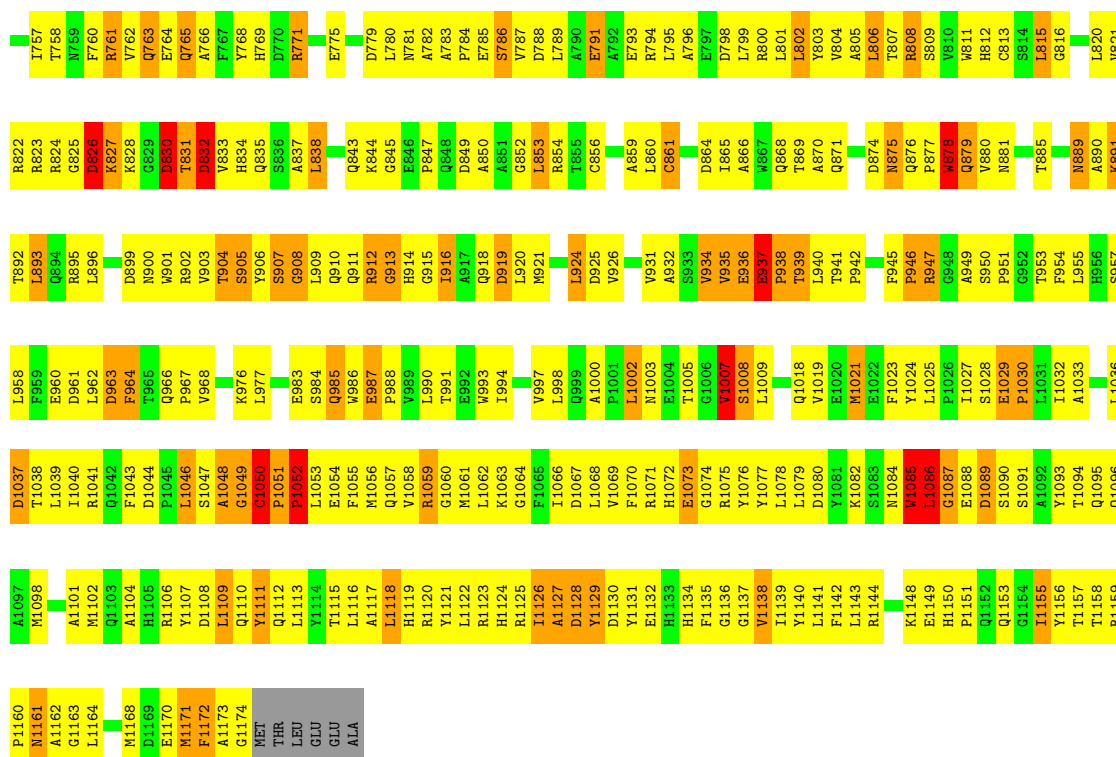
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0

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.

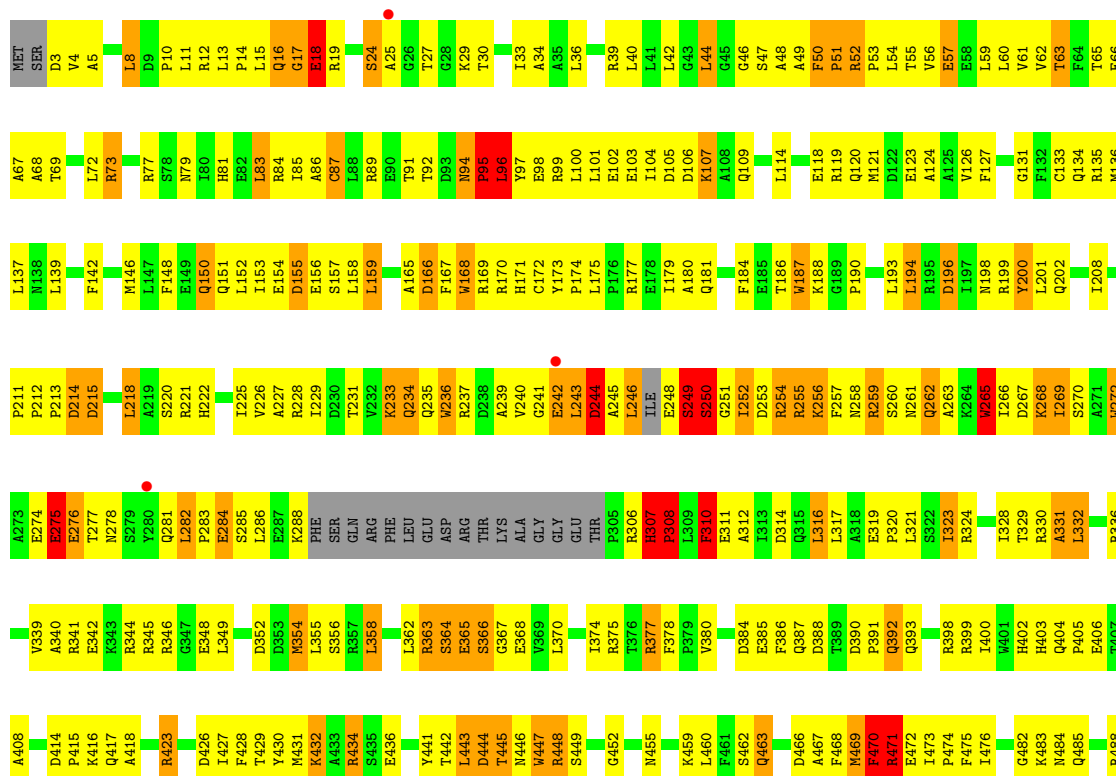
• Molecule 1: Exodeoxyribonuclease V beta chain

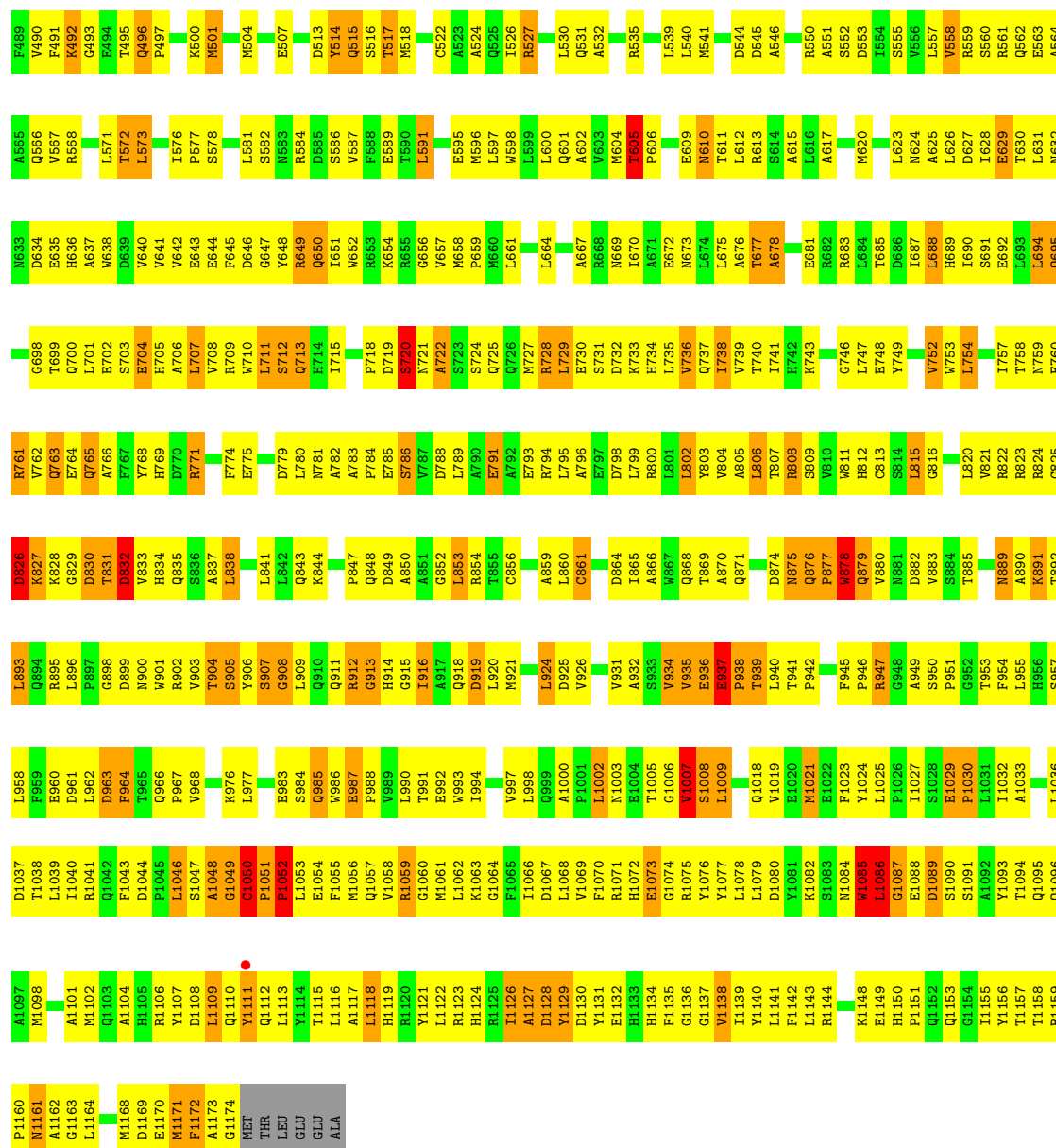




• Molecule 1: Exodeoxyribonuclease V beta chain

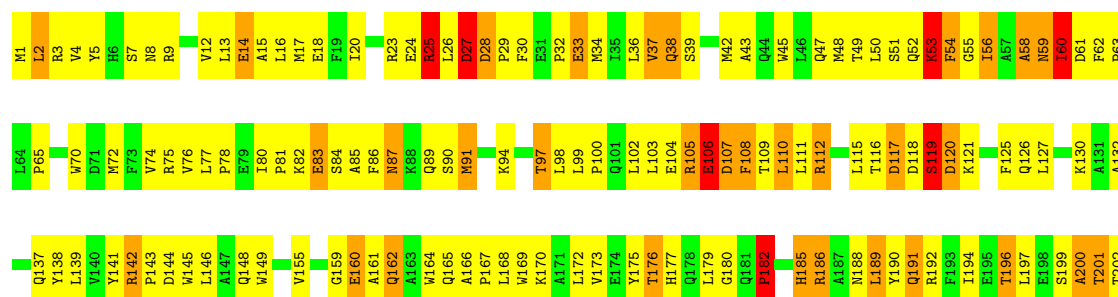
Chain E: 31% 51% 14% 2%

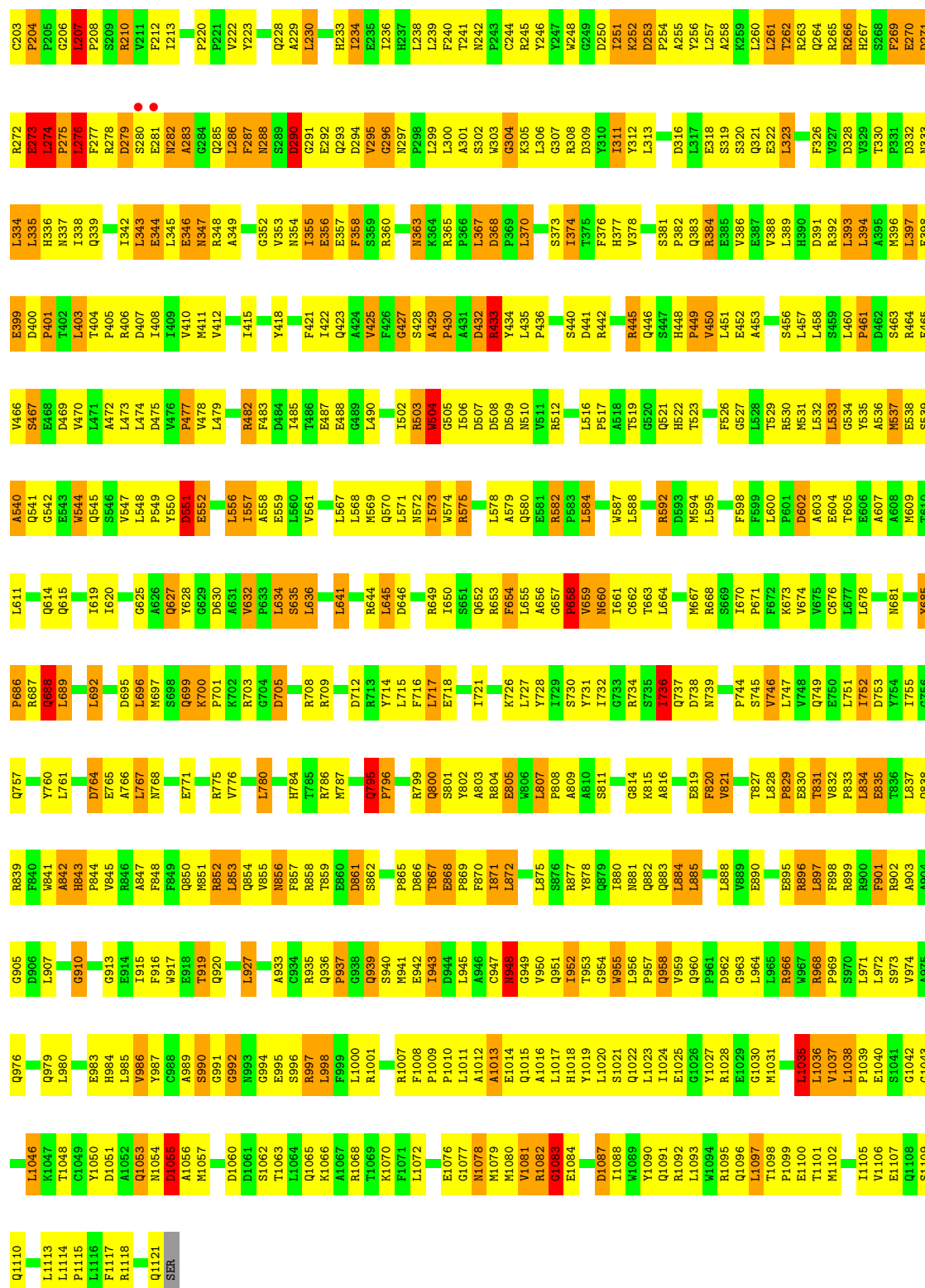




● Molecule 2: Exodeoxyribonuclease V gamma chain

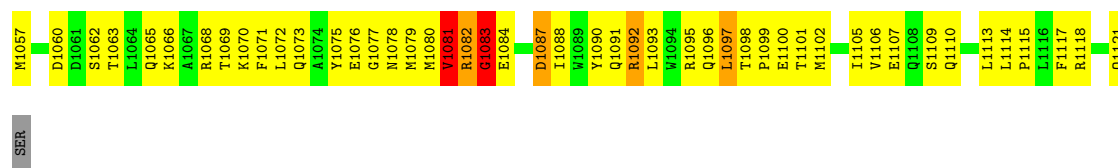
Chain C: 34% 48% 16%



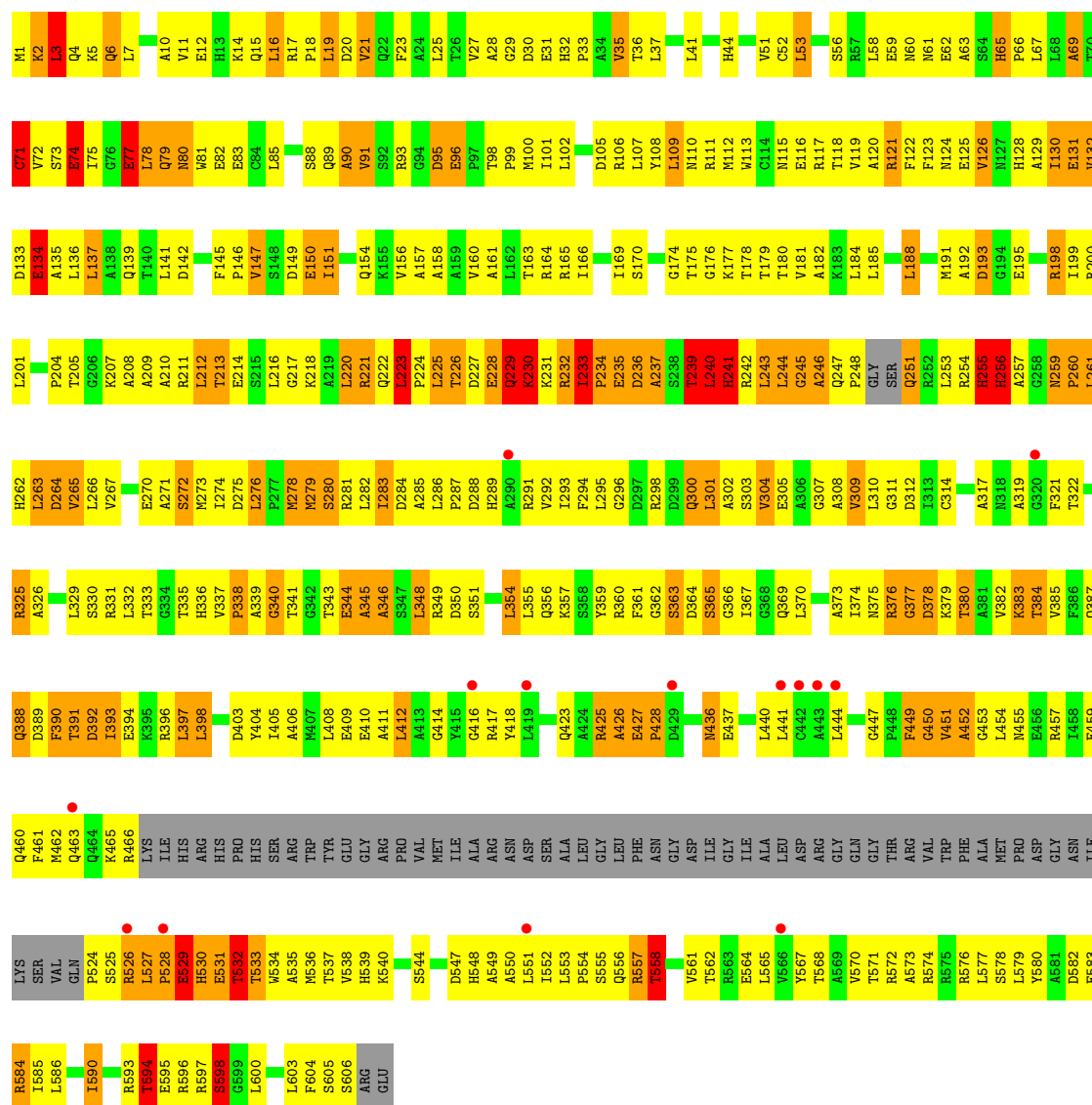


• Molecule 2: Exodeoxyribonuclease V gamma chain

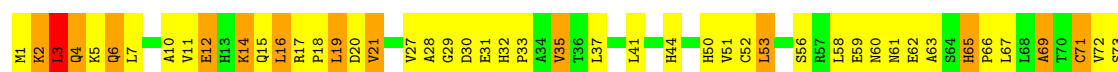
G992	R993	G994	E995	S996	R997	L998	F999	L1000	R1001	L1007	F1008	P1009	P1010	L1011	L1012	A1013	E1014	Q1015	A1016	L1017	H1018	Y1019	T1020	S1021	Q1022	L1023	P1024	E1025	Q1026	Y1027	R1028	G1029	L1030	M1031	S1032	A1033	F1034	L1035	V1036	L1038	P1039	E1040	S1041	G1042	G1043	L1046	T1047	C1048	H984	Y1050	D1051	L1052	Q1053	T1054	S990	L1055	A1056
F849	Q850	R851	R852	L853	Q854	R855	R856	F857	R858	S860	D861	S862	P865	R866	T867	E868	P869	F870	L871	L872	R877	Y878	Q879	R880	L881	Q882	Q883	L884	R885	L888	V889	E890	E895	R896	L897	R898	L899	R900	F901	G905	Y909	G910	A911	F912	G913	L915	Y916	Y917	E918	T919	Q920						
A766	L767	N768	C769	E771	R775	V776	L780	R786	N787	Q795	P796	R799	Q800	S801	Y802	A803	R804	E805	L806	L807	P808	Y809	L815	K816	E819	F820	V821	T827	L828	P829	E830	T831	V832	P833	L834	T836	Q837	Q838	Q839	F840	G842	A843	F844	V845	R846	T847	F848										
Q849	R850	R851	L852	R853	Q854	R855	R856	F857	R858	S840	R861	E862	P863	P865	D866	T867	E868	P869	F870	L871	L872	R877	Y878	Q879	R880	L881	R882	Q883	Q884	R885	L888	V889	E890	E895	R896	L897	R898	L899	R900	F901	G905	Y909	G910	A911	F912	G913	L915	Y916	Y917	E918	T919	Q920					
L927	A933	C934	R935	R936	Q937	G938	Q939	S940	M941	E942	I943	D944	L945	A946	C947	R948	Q949	V950	L951	Q952	T953	G954	W955	L956	Q957	Q958	L959	Q960	P961	D962	G963	L964	R965	R966	Q967	R968	P969	S970	L971	L972	R973	V974	Q976	Q979	L980	E983	H984	L985	Y986	D1051	Q1052	Q1053	T1054	S990	L1055	A1056	
A472	L473	L474	D475	V476	D477	A478	V479	R482	F483	D484	L485	T486	E487	E488	G489	L490	T502	R503	W504	S505	L506	D507	D508	D509	N510	V511	R512	L516	P517	A518	T519	G520	Q521	H522	T523	W524	R525	F526	G527	L528	T529	M530	M531	L532	L533	G534	Y535	A536	M537	A608	Q609	T610	L611	Q614	Q615	W544	
Q546	V547	L548	P549	V550	D551	E552	L556	I557	A558	E559	L560	V561	L567	L568	N569	Q570	N572	L573	O574	N575	N576	B577	L578	A579	Q580	E581	R582	P583	L584	N587	L588	R592	D593	M594	L595	F598	F599	L600	P601	D602	A603	E604	T605	E606	A607	A608	Q609	T610	L611	Q614	Q615	W544					
I619	I620	G625	A626	Q627	Y628	G629	D630	R631	P632	L633	S635	L636	L641	R644	L645	Q652	R653	F654	L655	A656	G657	Q658	V659	N660	L661	T662	L664	M667	I670	P671	F672	K673	V674	V675	C676	L677	L678	N681	Y685	P686	R687	Q688	L689	L692	D695	L696											
A472	L473	L474	D475	V476	D477	A478	V479	R482	F483	D484	L485	T486	E487	E488	G489	L490	T502	R503	W504	S505	L506	D507	D508	D509	N510	V511	R512	L516	P517	A518	T519	G520	Q521	H522	T523	W524	R525	F526	G527	L528	T529	M530	M531	L532	L533	G534	Y535	A536	M537	A608	Q609	T610	L611	Q614	Q615	W544	
L403	T404	P405	R406	D407	I408	L409	V410	M411	V412	L415	Y418	F421	I422	V425	F426	S428	A429	P430	A431	D432	R433	Y434	L435	S440	D441	R442	R445	Q446	S447	H448	P449	V450	L451	A452	A453	L455	S456	L457	L458	S459	L460	P461	R464	F465	V466	S467	E468	D469	V470	L471							
L273	L274	P275	L276	F277	R278	D279	S280	E281	N282	A283	Q285	L286	F287	N288	S289	D290	G291	E292	Q293	D294	V295	G296	N297	S302	W303	G304	K305	L306	G307	R308	P309	V310	H311	Y312	L313	D316	L317	E318	S319	S320	Q321	E322	L323	F326	V327	S328	D332	N333	K334	L335	H336	N337	D400	P401	T402		
G206	L207	P208	S209	R210	D211	F212	L213	P220	N221	V222	Y223	L224	Q225	Q228	A229	L230	H233	T234	E235	L236	W237	K238	L239	F240	E174	Y175	N242	P243	C244	R245	Y246	G248	G249	D250	T251	K252	D253	P254	A255	Y256	L257	A258	R259	L260	L261	T262	R263	Q264	R265	S266	H267	S268	F269	E270	D271	P205	
F68	I69	W70	D71	M72	F73	W74	R75	V76	L77	P78	E79	I80	P81	K82	S84	A85	F86	N87	S90	E91	W94	K94	T97	L98	F240	E174	Y175	N242	P243	C244	R245	Y246	G248	G249	D250	T251	K252	D253	P254	A255	Y256	L257	A258	R259	L260	L261	T262	R263	Q264	R265	S266	H267	S268	F269	E270	D271	P205
L139	V140	Y141	R142	P143	D144	W145	L146	W149	P221	V222	Y223	L224	Q225	Q228	A229	L230	H233	T234	E235	L236	W237	K238	L239	F240	E174	Y175	N242	P243	C244	R245	Y246	G248	G249	D250	T251	K252	D253	P254	A255	Y256	L257	A258	R259	L260	L261	T262	R263	Q264	R265	S266	H267	S268	F269	E270	D271	P205	
M1	L2	R3	V4	Y5	H6	S7	M8	R9	V12	L13	E14	A15	L16	M17	E18	F19	I20	R23	S90	E91	W94	K94	T97	L98	F240	E174	Y175	N242	P243	C244	R245	Y246	G248	G249	D250	T251	K252	D253	P254	A255	Y256	L257	A258	R259	L260	L261	T262	R263	Q264	R265	S266	H267	S268	F269	E270	D271	P205

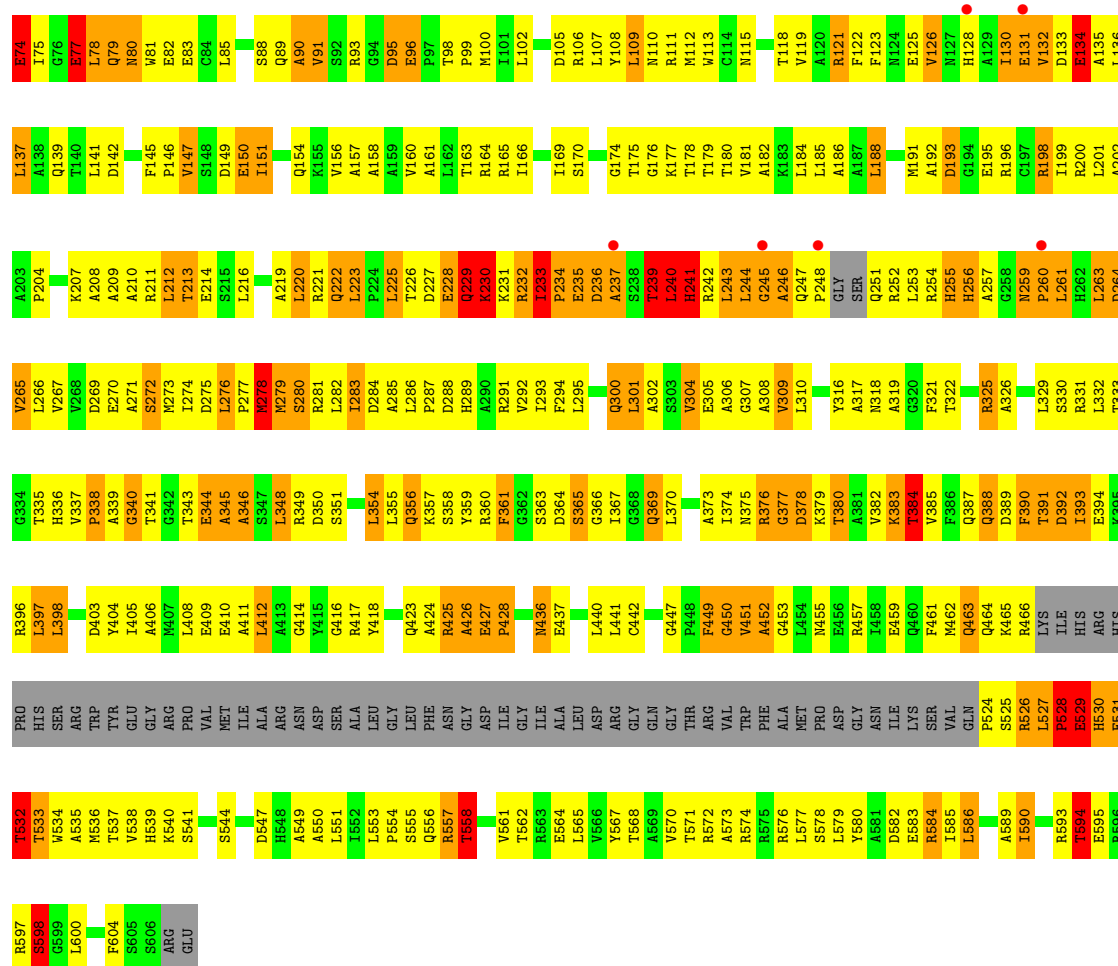


• Molecule 3: Exodeoxyribonuclease V alpha chain

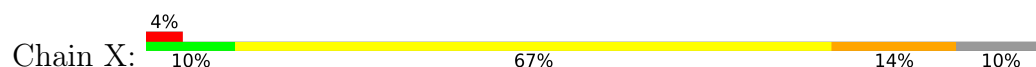


• Molecule 3: Exodeoxyribonuclease V alpha chain





• Molecule 4: DNA (46-MER)



• Molecule 4: DNA (46-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.80Å 192.90Å 334.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.59 30.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-3.59) 96.2 (30.00-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.296 0.237 , 0.280	Depositor DCC
R_{free} test set	4709 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 96.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46932	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: CA, 5IU

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	B	0.35	0/9432	1.08	68/12795 (0.5%)
1	E	0.35	0/9432	1.08	69/12795 (0.5%)
2	C	0.35	0/9305	1.03	72/12644 (0.6%)
2	F	0.35	0/9305	1.02	67/12644 (0.5%)
3	D	0.46	1/4281 (0.0%)	1.20	45/5796 (0.8%)
3	G	0.41	0/4281	1.17	44/5796 (0.8%)
4	X	0.33	0/847	0.79	4/1293 (0.3%)
4	Y	0.32	0/847	0.79	1/1293 (0.1%)
All	All	0.37	1/47730 (0.0%)	1.07	370/65056 (0.6%)

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
4	Y	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	255	HIS	N-CA	5.18	1.52	1.46

The worst 5 of 370 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	878	TRP	N-CA-C	-16.04	93.03	112.59
3	D	531	GLU	N-CA-C	-14.61	96.06	112.57
3	G	531	GLU	N-CA-C	-14.40	96.30	112.57
1	B	913	GLY	N-CA-C	-13.52	99.11	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	307	HIS	CA-C-N	13.52	136.74	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Y	10	DA	Sidechain

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	B	9236	0	9083	1020	0
1	E	9236	0	9083	969	0
2	C	9078	0	8877	891	0
2	F	9078	0	8877	859	0
3	D	4216	0	4261	614	0
3	G	4216	0	4261	599	0
4	X	935	0	498	114	0
4	Y	935	0	498	116	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	46932	0	45438	4933	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 53.

The worst 5 of 4933 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:205:THR:HA	4:X:3:5IU:OP1	1.39	1.21
1:B:442:THR:HG21	1:B:476:ILE:HD11	1.24	1.17
1:E:620:MET:HE3	1:E:687:ILE:HD13	1.27	1.16
4:X:22:DG:C2'	4:X:23:DC:H5''	1.75	1.16
3:D:65:HIS:HB3	3:D:66:PRO:HD2	1.20	1.15

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	B	1149/1180 (97%)	883 (77%)	173 (15%)	93 (8%)	1	8
1	E	1149/1180 (97%)	885 (77%)	173 (15%)	91 (8%)	1	8
2	C	1119/1122 (100%)	870 (78%)	164 (15%)	85 (8%)	1	9
2	F	1119/1122 (100%)	870 (78%)	162 (14%)	87 (8%)	1	8
3	D	541/608 (89%)	374 (69%)	97 (18%)	70 (13%)	0	3
3	G	541/608 (89%)	375 (69%)	95 (18%)	71 (13%)	0	3
All	All	5618/5820 (96%)	4257 (76%)	864 (15%)	497 (9%)	0	7

5 of 497 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	GLY
1	B	18	GLU
1	B	95	PRO
1	B	96	LEU
1	B	155	ASP

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	B	978/999 (98%)	838 (86%)	140 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	978/999 (98%)	839 (86%)	139 (14%)	3	19
2	C	976/977 (100%)	828 (85%)	148 (15%)	3	17
2	F	976/977 (100%)	825 (84%)	151 (16%)	2	16
3	D	443/492 (90%)	374 (84%)	69 (16%)	2	16
3	G	443/492 (90%)	377 (85%)	66 (15%)	3	17
All	All	4794/4936 (97%)	4081 (85%)	713 (15%)	3	17

5 of 713 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	838	LEU
2	F	557	ILE
1	E	958	LEU
1	E	832	ASP
2	F	183	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 278 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	699	GLN
2	F	812	GLN
3	G	22	GLN
2	C	800	GLN
2	C	792	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
4	5IU	X	7	4	18,21,22	0.50	0	25,30,33	0.89	1 (4%)
4	5IU	X	50	4	18,21,22	0.51	0	25,30,33	0.47	0
4	5IU	Y	4	4	18,21,22	0.40	0	25,30,33	0.46	0
4	5IU	X	3	4	18,21,22	0.48	0	25,30,33	0.74	0
4	5IU	Y	7	4	18,21,22	0.52	0	25,30,33	0.93	1 (4%)
4	5IU	Y	1	4	18,18,22	0.52	0	26,26,33	0.35	0
4	5IU	X	9	4	18,21,22	0.69	1 (5%)	25,30,33	0.42	0
4	5IU	X	5	4	18,21,22	1.76	4 (22%)	25,30,33	0.77	0
4	5IU	Y	2	4	18,21,22	0.56	0	25,30,33	0.75	1 (4%)
4	5IU	X	2	4	18,21,22	0.51	0	25,30,33	0.66	1 (4%)
4	5IU	Y	46	4	18,21,22	0.46	0	25,30,33	0.59	0
4	5IU	X	1	4	18,18,22	0.54	0	26,26,33	0.34	0
4	5IU	X	46	4	18,21,22	0.52	0	25,30,33	0.71	0
4	5IU	Y	3	4	18,21,22	0.41	0	25,30,33	0.76	0
4	5IU	Y	5	4	18,21,22	0.60	0	25,30,33	0.94	1 (4%)
4	5IU	X	4	4	18,21,22	0.48	0	25,30,33	0.44	0
4	5IU	Y	9	4	18,21,22	0.63	0	25,30,33	0.42	0
4	5IU	Y	50	4	18,21,22	0.45	0	25,30,33	0.47	0

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
4	5IU	X	7	4	-	0/7/21/22	0/2/2/2
4	5IU	X	50	4	-	5/7/21/22	0/2/2/2
4	5IU	Y	4	4	-	6/7/21/22	0/2/2/2
4	5IU	X	3	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	7	4	-	0/7/21/22	0/2/2/2
4	5IU	Y	1	4	-	2/6/18/22	0/2/2/2
4	5IU	X	9	4	-	0/7/21/22	0/2/2/2
4	5IU	X	5	4	-	6/7/21/22	0/2/2/2
4	5IU	Y	2	4	-	2/7/21/22	0/2/2/2
4	5IU	X	2	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	46	4	-	3/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5IU	X	1	4	-	2/6/18/22	0/2/2/2
4	5IU	X	46	4	-	3/7/21/22	0/2/2/2
4	5IU	Y	3	4	-	2/7/21/22	0/2/2/2
4	5IU	Y	5	4	-	6/7/21/22	0/2/2/2
4	5IU	X	4	4	-	6/7/21/22	0/2/2/2
4	5IU	Y	9	4	-	0/7/21/22	0/2/2/2
4	5IU	Y	50	4	-	6/7/21/22	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	5	5IU	O2-C2	5.38	1.32	1.23
4	X	5	5IU	C6-N1	3.65	1.44	1.38
4	X	5	5IU	C2-N1	2.23	1.42	1.38
4	X	5	5IU	O4-C4	2.04	1.27	1.23
4	X	9	5IU	C5-I5	-2.02	2.02	2.08

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	7	5IU	C2'-C1'-N1	-2.90	106.57	113.81
4	Y	5	5IU	C2'-C1'-N1	-2.85	106.67	113.81
4	X	7	5IU	C2'-C1'-N1	-2.81	106.80	113.81
4	Y	2	5IU	C2'-C1'-N1	-2.22	108.27	113.81
4	X	2	5IU	C2'-C1'-N1	-2.21	108.30	113.81

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	X	1	5IU	O4'-C1'-N1-C2
4	X	1	5IU	O4'-C1'-N1-C6
4	X	2	5IU	O4'-C1'-N1-C2
4	X	2	5IU	O4'-C1'-N1-C6
4	X	5	5IU	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	7	5IU	6	0
4	X	50	5IU	1	0
4	Y	4	5IU	4	0
4	X	3	5IU	12	0
4	Y	7	5IU	9	0
4	Y	1	5IU	3	0
4	X	9	5IU	6	0
4	X	5	5IU	3	0
4	Y	2	5IU	14	0
4	X	2	5IU	15	0
4	Y	46	5IU	11	0
4	X	1	5IU	1	0
4	X	46	5IU	11	0
4	Y	3	5IU	13	0
4	Y	5	5IU	1	0
4	X	4	5IU	6	0
4	Y	9	5IU	8	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	B	1155/1180 (97%)	-0.26	4 (0%) 90 75	54, 111, 179, 259	0
1	E	1155/1180 (97%)	-0.23	4 (0%) 90 75	59, 121, 179, 215	0
2	C	1121/1122 (99%)	-0.32	2 (0%) 91 80	42, 90, 155, 226	0
2	F	1121/1122 (99%)	-0.27	3 (0%) 90 75	54, 107, 172, 222	0
3	D	547/608 (89%)	0.23	14 (2%) 57 33	71, 165, 222, 251	0
3	G	547/608 (89%)	-0.09	6 (1%) 78 52	55, 114, 188, 243	0
4	X	37/51 (72%)	0.52	2 (5%) 31 18	82, 168, 227, 236	0
4	Y	37/51 (72%)	0.29	0 100 100	106, 168, 222, 247	0
All	All	5720/5922 (96%)	-0.20	35 (0%) 85 64	42, 112, 190, 259	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	245	ALA	3.5
1	E	1111	TYR	3.4
4	X	10	DA	3.2
1	B	285	SER	3.0
1	E	280	TYR	3.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
4	5IU	Y	1	17/21	0.21	0.18	234,234,300,300	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	5IU	X	1	17/21	0.46	0.13	200,200,300,300	0
4	5IU	X	2	20/21	0.53	0.19	108,164,275,275	0
4	5IU	X	5	20/21	0.57	0.15	108,156,300,300	0
4	5IU	Y	5	20/21	0.66	0.15	108,300,300,300	0
4	5IU	Y	7	20/21	0.66	0.14	108,181,300,300	0
4	5IU	Y	4	20/21	0.68	0.14	108,300,300,300	0
4	5IU	Y	50	20/21	0.69	0.12	108,170,300,300	0
4	5IU	Y	2	20/21	0.71	0.15	108,300,300,300	0
4	5IU	X	3	20/21	0.74	0.13	108,179,254,254	0
4	5IU	X	50	20/21	0.74	0.15	108,155,260,260	0
4	5IU	X	7	20/21	0.76	0.13	108,158,216,216	0
4	5IU	Y	46	20/21	0.81	0.12	108,158,252,252	0
4	5IU	X	46	20/21	0.82	0.13	108,165,189,189	0
4	5IU	X	4	20/21	0.84	0.10	108,140,235,235	0
4	5IU	Y	3	20/21	0.86	0.13	108,300,300,300	0
4	5IU	Y	9	20/21	0.90	0.10	102,108,148,148	0
4	5IU	X	9	20/21	0.96	0.10	58,108,124,124	0

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
5	CA	B	4000	1/1	0.95	0.07	108,108,108,108	0
5	CA	E	4000	1/1	0.98	0.04	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.