



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:28 PM UTC

PDB ID : 1W36 / pdb_00001w36
Title : RecBCD:DNA complex
Authors : Singleton, M.R.; Dillingham, M.S.; Gaudier, M.; C Kowalczykowski, S.;
Wigley, D.B.
Deposited on : 2004-07-13
Resolution : 3.10 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
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

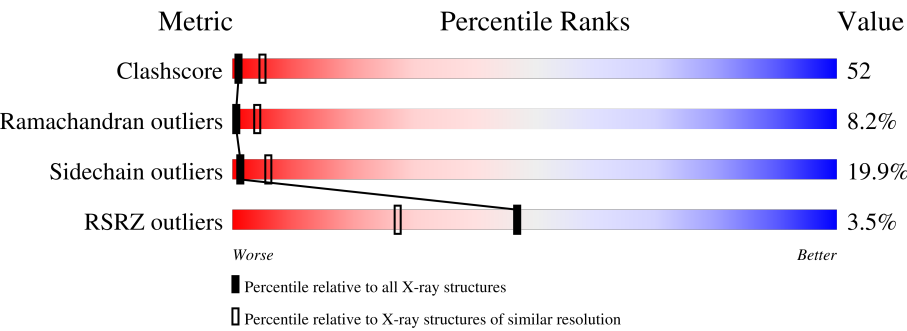
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	3% 28% 45% 21%
1	E	1180	3% 30% 45% 20%
2	C	1122	% 31% 44% 20%
2	F	1122	% 34% 40% 18%
3	D	608	4% 26% 39% 19%
3	G	608	12% 25% 41% 19%
4	Y	43	2% 12% 65% 9%

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Mol	Chain	Length	Quality of chain
4	Z	43	5% 14% 65% 9% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 46145 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	1158	Total	C	N	O	S	0	0	0
			9258	5837	1641	1740	40			
1	E	1158	Total	C	N	O	S	0	0	0
			9258	5837	1641	1740	40			

- Molecule 2 is a protein called EXODEOXYRIBONUCLEASE V GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1122	Total	C	N	O	S	0	0	1
			9079	5783	1569	1684	43			
2	F	1078	Total	C	N	O	S	0	0	1
			8714	5558	1501	1612	43			

- Molecule 3 is a protein called EXODEOXYRIBONUCLEASE V ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	539	Total	C	N	O	S	0	0	1
			4144	2587	754	785	18			
3	G	539	Total	C	N	O	S	0	0	1
			4144	2587	754	785	18			

- Molecule 4 is a DNA chain called DNA HAIRPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	38	Total	C	N	O	P	0	0	0
			773	371	142	224	36			
4	Z	38	Total	C	N	O	P	0	0	0
			773	371	142	224	36			

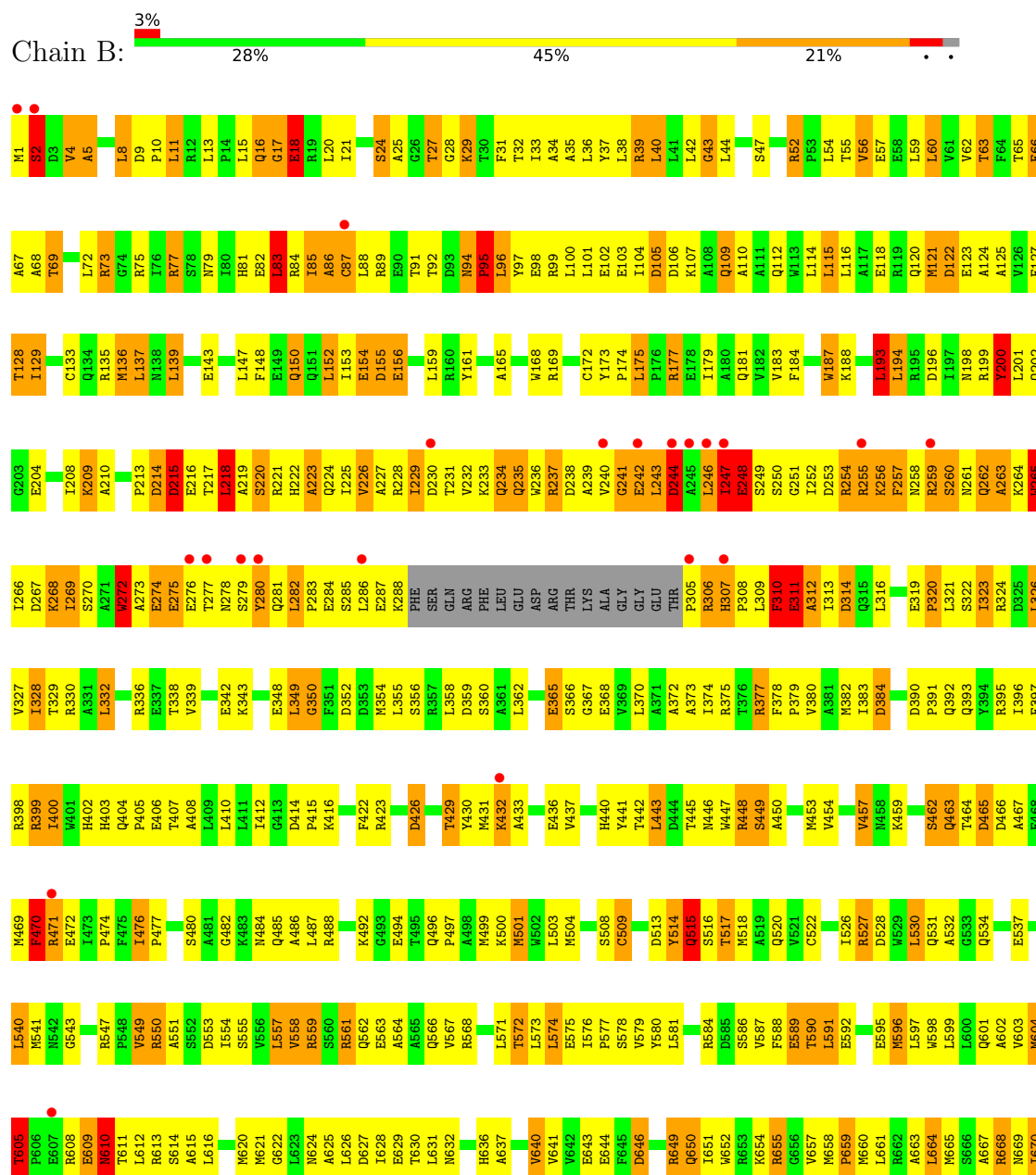
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

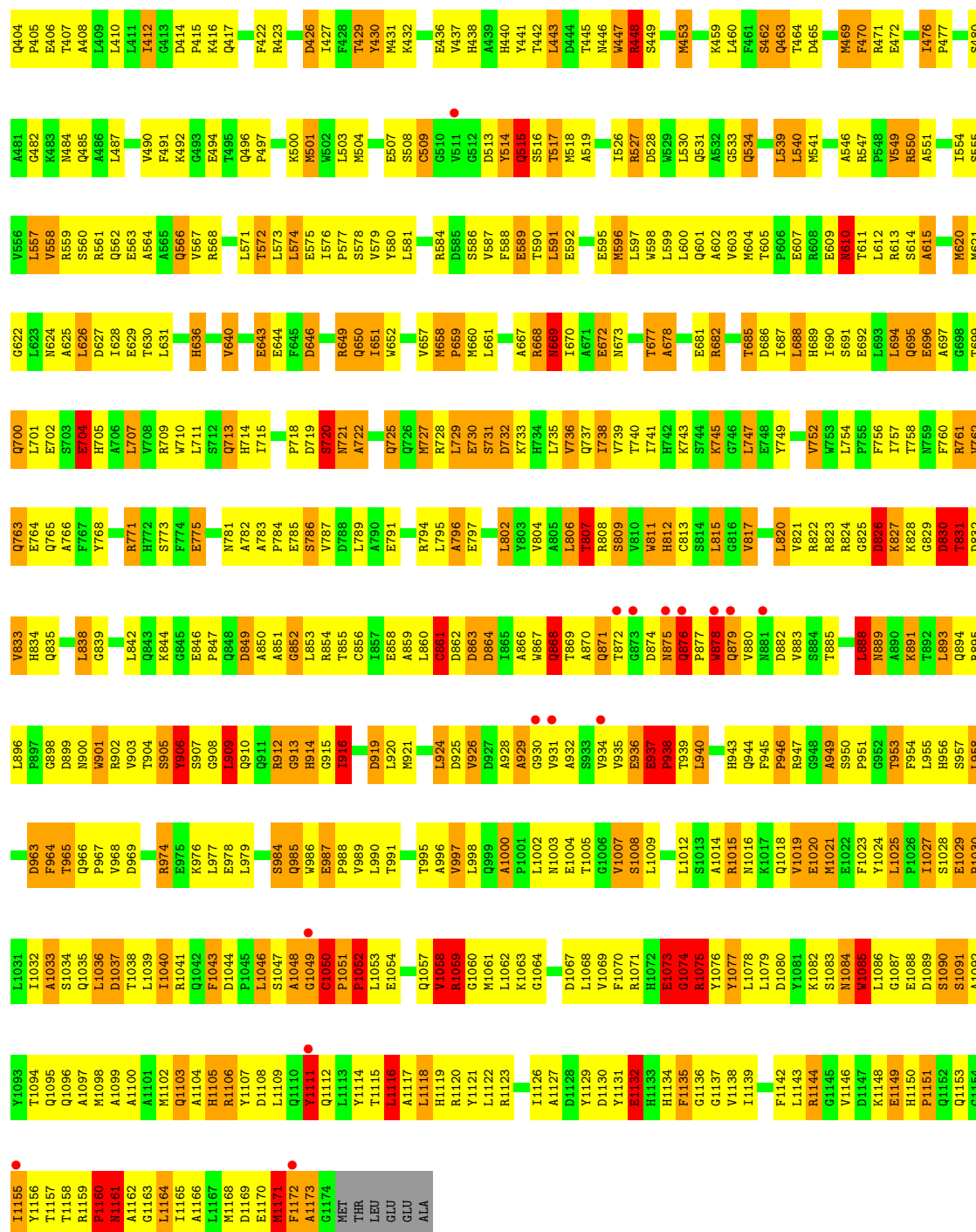
3 Residue-property plots

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.

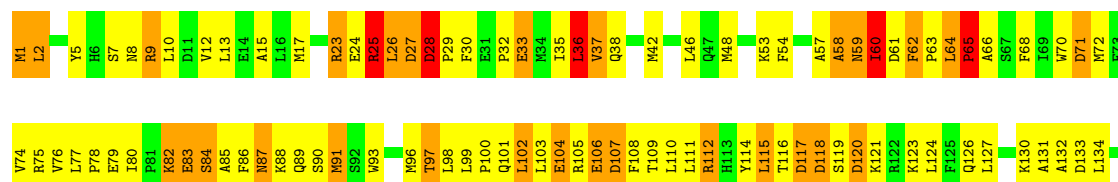
• Molecule 1: EXODEOXYRIBONUCLEASE V BETA CHAIN





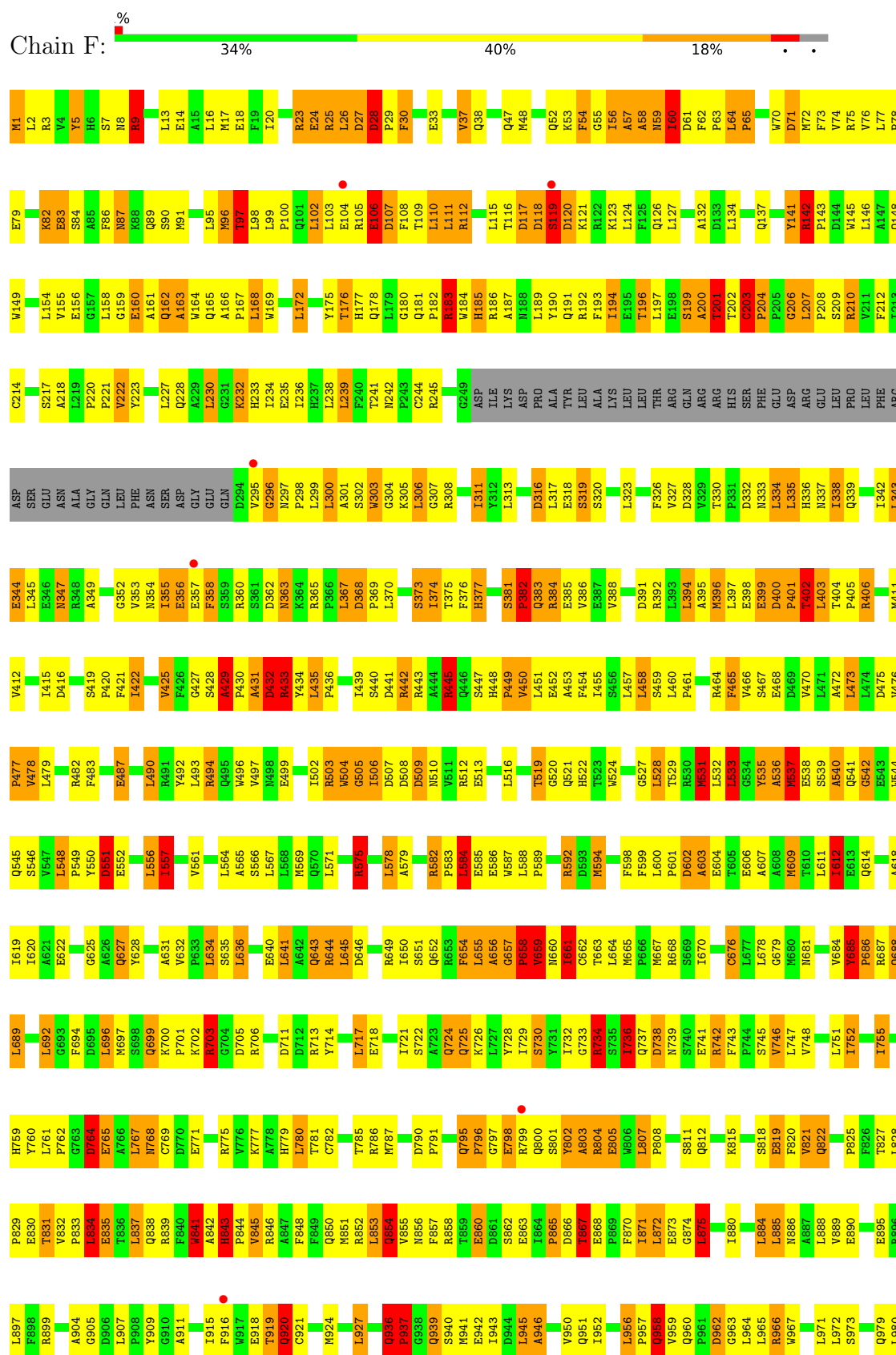


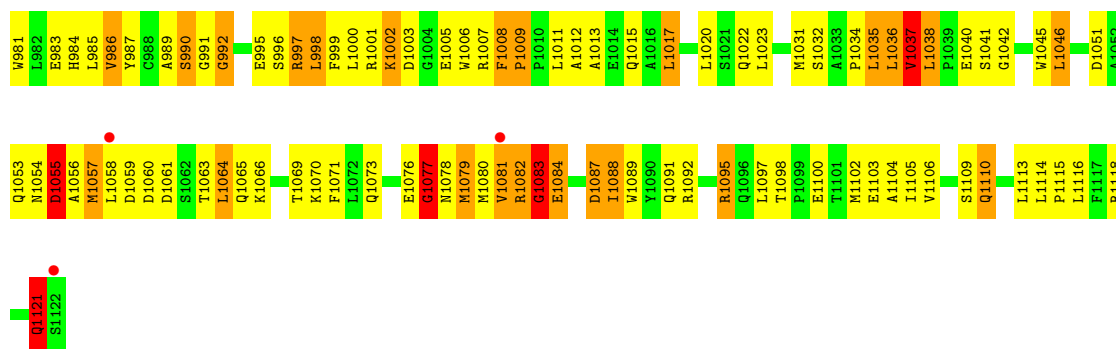
Chain C: 31% 44% 20%



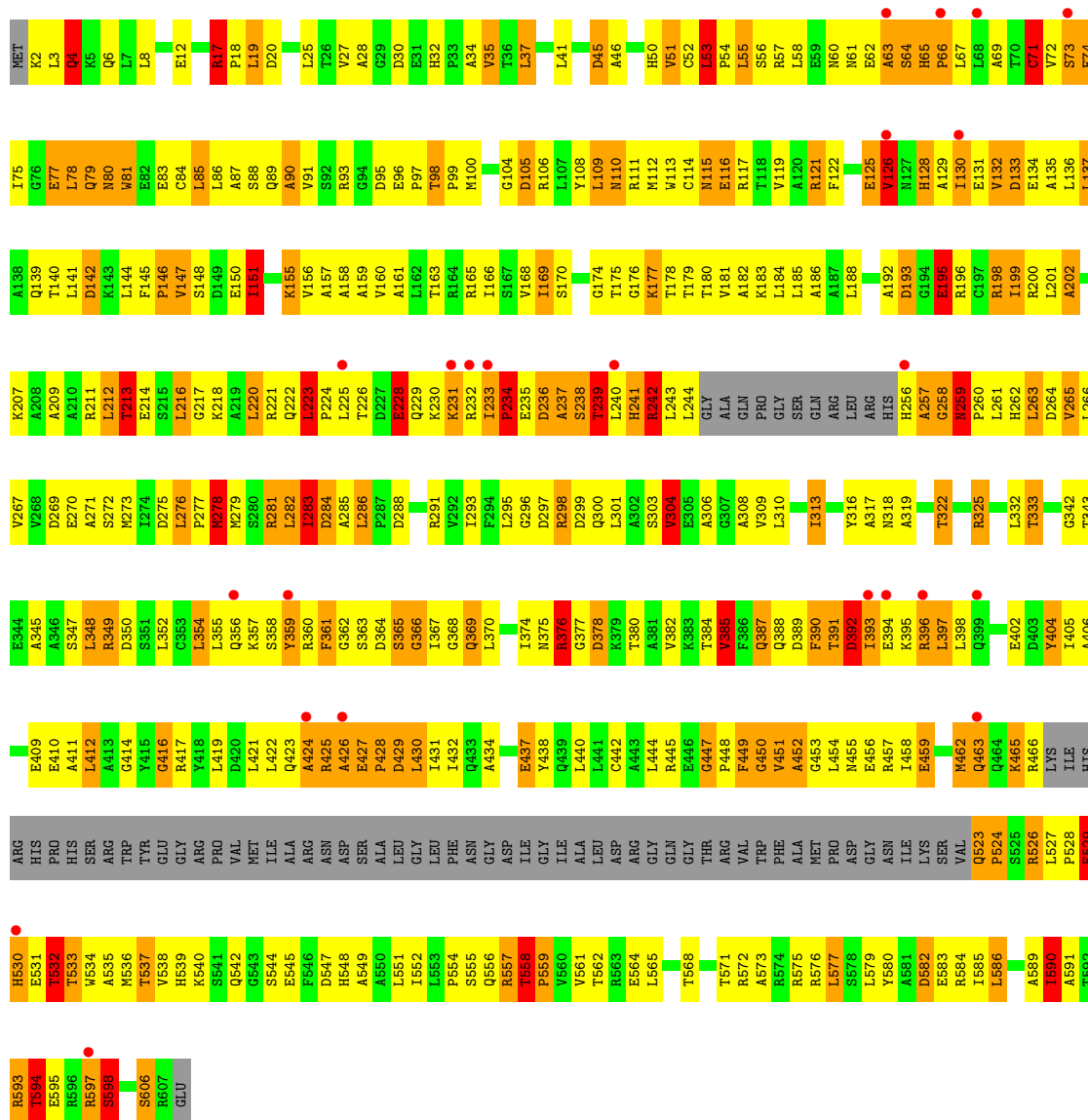
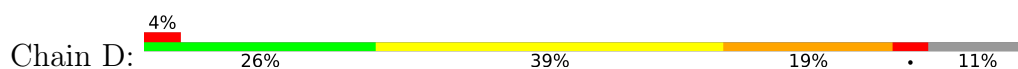
L1097	Q1026	L964	N886	P825	L747	D682	I612	E543	L473	L403	L336	D271	T202	Q137
T1098	Y1027	L965	V889	F826	V748	G883	E613	W544	L474	T404	H336	R272	C203	Y138
P1099	M1031	L966	E889	T827	Q749	Y684	Q614	Q545	D475	P405	N337	E273	P204	L139
E1100	M1031	E890	E890	L828	Q750	Y685	Q614	Q545	D476	P406	L338	L274	V140	V140
T1101	P1034	R968	Q891	P829	L751	P686	A618	L548	P477	D407	Q339	P275	L207	R142
E1103	L1035	S970	E895	E830	I752	R687	I619	P549	V478	L408	S340	L276	P208	P143
A1104	L1036	L971	R896	T831	I755	G888	I620	Y550	L479	T409	D341	F277	S209	
L1105	L1037	L972	R897	V832	I755	A890	A621	D551	R482	V410	L342	R278	R210	L146
V1106	L1038	S973	F898	L834	Y760	P691	G623	Q552	F483	N411	E344	D279	V211	A147
E1107	P1039	S973	R899	E835	Y760	P691	G623	Q552	D484	V412	E344	E280	T212	Q148
Q1108	E1040	Q976	R902	T836	L761	G693	G625	L556	L485	L415	E346	N282	C214	W149
S1109	S1041	Q977	R902	T837	P762	F694	A626	A558	Y486	L418	R347	A283	P220	L154
R1110	A1044	Q978	Y909	Q838	G763	D695	Q627	E559	E487	Y418	R346	Q285	P221	V155
F1112	W1045	Q979	R839	R839	G764	Y628	Y628	L560	E488	S419	A349	Q285	V222	E156
L1113	L1046	Q980	G910	F840	D765	R696	G629	V561	D489	P420	L286	Y223	Y223	G157
L1114	L1046	Q981	A911	W841	A766	S698	D630	G562	L490	F421	G352	F287	Y223	L158
L1115	D1061	L982	A842	A842	L767	Q699	G563	G564	L493	L422	V353	N288	A226	G159
L1116	A1062	E983	H843	H843	N768	K700	V632	L564	L494	V425	R356	D290	L227	E160
Q1063	Q1063	H984	P844	P844	C769	P701	F633	A565	R494	F426	R365	D291	Q228	A161
L1064	Q1065	L985	V845	V845	D770	R703	S635	S566	E499	Q427	E357	E292	A229	Q162
L1065	D1065	Y987	A847	A847	G704	G704	L636	L568	S428	S428	F358	Q293	L230	A163
A1066	A1066	Q988	F848	F848	D705	D705	E640	Q570	L502	P430	S359	D294	G231	W164
M1067	M1067	L899	L899	L899	L780	R706	E641	Q571	L504	A431	R360	V295	K232	Q165
L1068	L1068	S990	L927	M851	G782	T781	L641	L571	L504	A431	R360	V295	K232	W165
L1069	L1069	G991	L927	M851	G782	T781	L641	L571	L504	A431	R360	V295	K232	A166
D1060	D1060	G992	L927	M851	G782	T781	L641	L571	L504	A431	R360	V295	K232	L168
L1061	S1061	E995	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	W169
D1062	D1062	E996	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	
T1063	T1063	E997	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	
L1064	L1064	E998	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	
Q1065	Q1065	E999	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	
L1066	L1066	E1000	V931	R852	D712	D712	Q642	N572	G505	D432	R363	N297	T241	
F1071	F1071	R1001	Q936	Q936	A718	A718	F654	Q580	E513	A444	L370	G307	R245	L172
L1072	L1072	R1002	Q936	Q936	A718	A718	F654	Q580	E513	A444	L370	G307	R245	V173
Q1073	Q1073	D1003	S940	S940	E798	E798	G657	P583	L516	F454	F376	R308	Y246	E174
A1074	A1074	E1004	L841	L841	R799	R799	P658	L584	T519	H448	F376	R308	Y246	Y175
E1075	E1075	E1005	E942	E942	Q800	Q800	V659	E585	G520	P449	F376	R308	Y246	H177
G1076	G1076	W1006	I943	I943	S801	S801	N660	E586	G521	V450	F376	R308	Y246	Q178
L1077	L1077	F1007	D944	D944	Y902	Y902	I661	V587	H522	L451	F376	R308	Y246	L179
M1078	M1078	F1008	L945	L945	A803	A803	C662	L588	T523	R452	F376	R308	Y246	G180
M1079	M1079	P1009	A946	A946	R804	R804	T663	P589	H524	A453	F376	R308	Y246	L181
M1080	M1080	F1010	A946	A946	R804	R804	T663	P589	H524	A453	F376	R308	Y246	P182
V1081	V1081	L1011	G949	G949	W806	W806	M665	C591	G527	L457	F376	R308	Y246	R183
R1082	R1082	A1012	V950	V950	L807	L807	P666	R592	L528	L458	F376	R308	Y246	W184
G1083	G1083	A1013	Q951	Q951	E874	E874	P667	D593	L532	L460	F376	R308	Y246	R186
E1084	E1084	E1014	I952	I952	G874	G874	M667	D594	L532	L460	F376	R308	Y246	A187
G1085	G1085	Q1015	T953	T953	L875	L875	R668	M594	L532	L460	F376	R308	Y246	N188
D1086	D1086	A1016	G954	G954	S876	S876	S669	L532	L532	L460	F376	R308	Y246	L189
L1087	L1087	L1017	W955	W955	R877	R877	F672	F598	L532	L460	F376	R308	Y246	Y190
I1088	I1088	H1018	L956	L956	Y878	Y878	K673	G534	L532	L460	F376	R308	Y246	Q191
W1089	W1089	Y1019	P957	P957	Q879	Q879	N739	Y535	L532	L460	F376	R308	Y246	R192
L1090	L1090	L1020	Q958	Q958	I880	I880	C676	A603	L532	L460	F376	R308	Y246	I194
S1021	S1021	S1021	V959	V959	N881	N881	L677	A603	L532	L460	F376	R308	Y246	E195
Q1092	Q1092	Q1092	Q960	Q960	Q882	Q882	L678	E604	L532	L460	F376	R308	Y246	L196
R1093	R1093	R1093	P961	P961	Q883	Q883	L679	E604	L532	L460	F376	R308	Y246	T197
L1094	L1094	L1023	D962	D962	L884	L884	M680	M609	L532	L460	F376	R308	Y246	E198
R1095	R1095	E1025	Q1096	Q1096	L885	L885	N881	M609	L532	L460	F376	R308	Y246	S199

● Molecule 2: EXODEOXYRIBONUCLEASE V GAMMA CHAIN

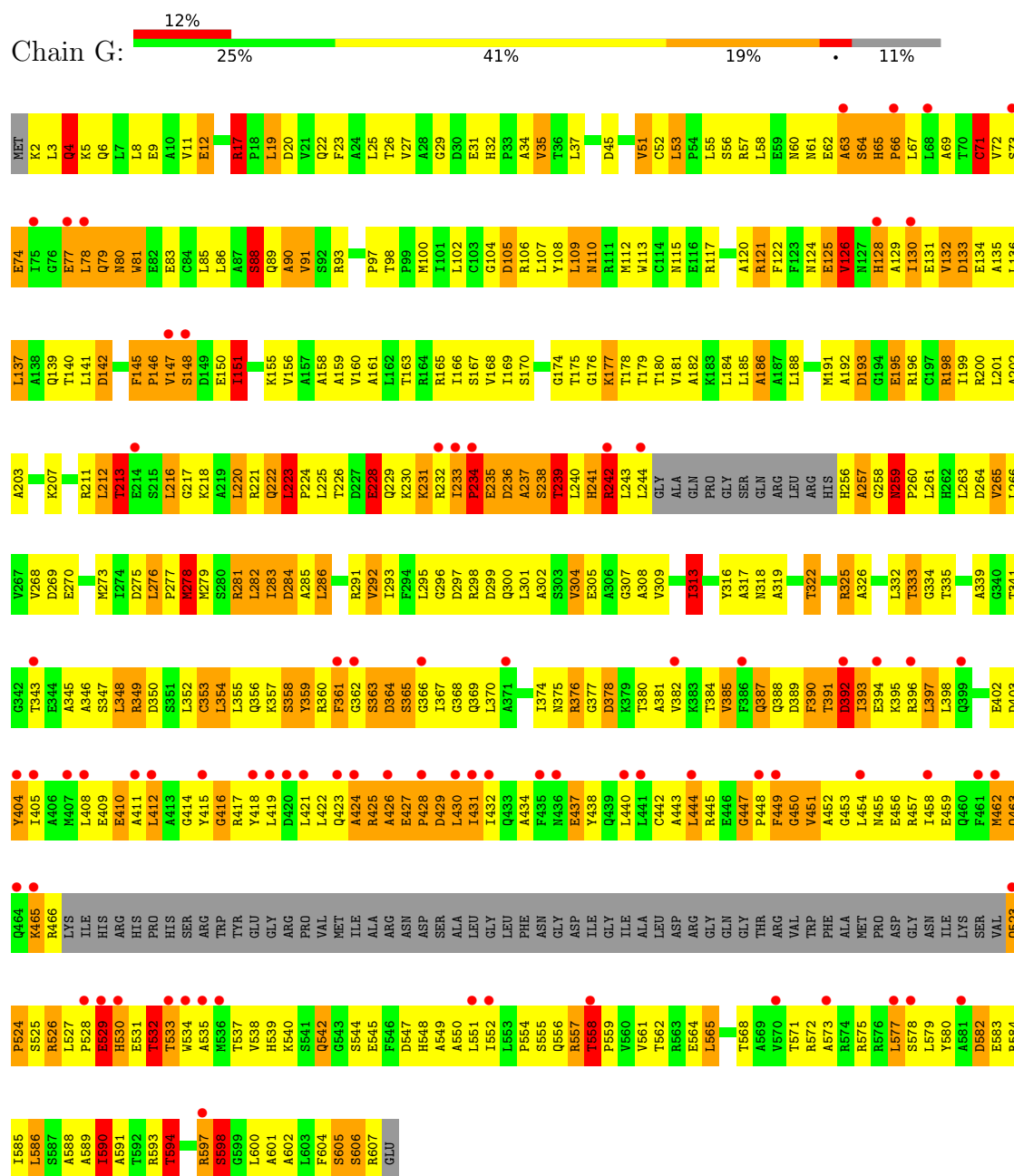




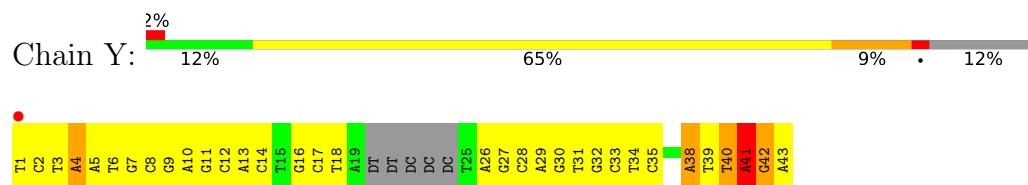
• Molecule 3: EXODEOXYRIBONUCLEASE V ALPHA CHAIN



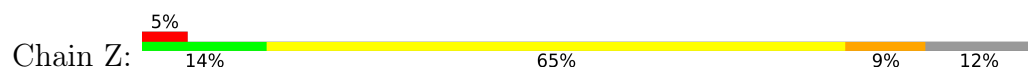
• Molecule 3: EXODEOXYRIBONUCLEASE V ALPHA CHAIN

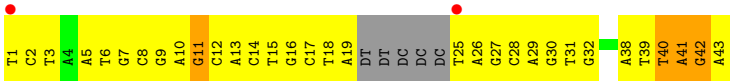


• Molecule 4: DNA HAIRPIN



• Molecule 4: DNA HAIRPIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.60Å 187.23Å 335.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.84 – 3.10 46.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.84-3.10) 99.9 (46.84-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.91 (at 3.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.296 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	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	0.91	EDS
Total number of atoms	46145	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% 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

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	0.95	7/9455 (0.1%)	1.44	161/12827 (1.3%)
1	E	1.05	12/9455 (0.1%)	1.45	164/12827 (1.3%)
2	C	1.02	13/9306 (0.1%)	1.47	158/12646 (1.2%)
2	F	1.23	31/8933 (0.3%)	1.51	173/12143 (1.4%)
3	D	0.95	7/4207 (0.2%)	1.49	77/5699 (1.4%)
3	G	0.95	7/4207 (0.2%)	1.47	81/5699 (1.4%)
4	Y	0.48	0/866	0.98	5/1333 (0.4%)
4	Z	0.46	0/866	1.00	7/1333 (0.5%)
All	All	1.03	77/47295 (0.2%)	1.45	826/64507 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	E	0	2
2	C	0	4
2	F	0	2
4	Y	0	2
All	All	0	12

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	665	MET	SD-CE	8.70	2.01	1.79
2	F	1	MET	SD-CE	8.47	2.00	1.79
2	F	609	MET	SD-CE	8.21	2.00	1.79
3	D	278	MET	SD-CE	7.85	1.99	1.79
2	F	866	ASP	CB-CG	7.70	1.71	1.52

The worst 5 of 826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1008	PHE	CA-C-N	18.27	132.99	119.66
2	F	1008	PHE	C-N-CA	18.27	132.99	119.66
3	G	531	GLU	N-CA-C	-18.05	92.18	112.57
3	D	531	GLU	N-CA-C	-17.68	94.23	112.97
1	E	1050	CYS	CA-C-N	-16.96	102.91	120.38

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	200	TYR	Sidechain
1	B	906	TYR	Sidechain
2	C	418	TYR	Sidechain
2	C	535	TYR	Sidechain
2	C	685	TYR	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	9258	0	9112	1092	0
1	E	9258	0	9112	991	0
2	C	9079	0	8877	979	0
2	F	8714	0	8528	763	1
3	D	4144	0	4181	469	0
3	G	4144	0	4181	446	0
4	Y	773	0	432	96	0
4	Z	773	0	432	87	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	46145	0	44855	4719	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

The worst 5 of 4719 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:1050:CYS:C	1:B:1052:PRO:HD2	1.63	1.23
1:E:1050:CYS:C	1:E:1052:PRO:HD2	1.64	1.23
4:Y:16:DG:C2'	4:Y:17:DC:H5''	1.69	1.21
2:C:442:ARG:HG3	2:C:442:ARG:HH11	1.05	1.18
3:G:62:GLU:HA	3:G:65:HIS:HB2	1.22	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:ARG:O	2:F:937:PRO:O[3_645]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1154/1180 (98%)	898 (78%)	164 (14%)	92 (8%)	1	4
1	E	1154/1180 (98%)	915 (79%)	147 (13%)	92 (8%)	1	4
2	C	1120/1122 (100%)	873 (78%)	164 (15%)	83 (7%)	1	5
2	F	1074/1122 (96%)	869 (81%)	135 (13%)	70 (6%)	1	6
3	D	533/608 (88%)	390 (73%)	81 (15%)	62 (12%)	0	1
3	G	533/608 (88%)	386 (72%)	90 (17%)	57 (11%)	0	2
All	All	5568/5820 (96%)	4331 (78%)	781 (14%)	456 (8%)	0	4

5 of 456 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	GLY
1	B	95	PRO
1	B	155	ASP
1	B	214	ASP

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Mol	Chain	Res	Type
1	B	244	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	B	981/999 (98%)	777 (79%)	204 (21%)	1	5
1	E	981/999 (98%)	782 (80%)	199 (20%)	1	5
2	C	976/977 (100%)	781 (80%)	195 (20%)	1	6
2	F	937/977 (96%)	758 (81%)	179 (19%)	1	7
3	D	436/492 (89%)	349 (80%)	87 (20%)	1	6
3	G	436/492 (89%)	355 (81%)	81 (19%)	1	8
All	All	4747/4936 (96%)	3802 (80%)	945 (20%)	1	6

5 of 945 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	380	THR
3	G	142	ASP
1	E	561	ARG
3	G	91	VAL
2	F	734	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 283 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	699	GLN
2	F	792	GLN
2	F	1121	GLN
2	C	737	GLN
2	C	688	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	B	1158/1180 (98%)	0.19	38 (3%)	49	29	31, 68, 111, 125	0
1	E	1158/1180 (98%)	0.07	36 (3%)	51	30	25, 56, 118, 140	0
2	C	1122/1122 (100%)	0.01	13 (1%)	76	58	30, 62, 103, 134	0
2	F	1078/1122 (96%)	-0.31	9 (0%)	82	65	22, 43, 76, 108	0
3	D	539/608 (88%)	0.30	23 (4%)	40	22	34, 70, 110, 127	0
3	G	539/608 (88%)	0.67	76 (14%)	6	3	32, 84, 135, 140	0
4	Y	38/43 (88%)	0.56	1 (2%)	57	36	68, 116, 152, 157	0
4	Z	38/43 (88%)	0.75	2 (5%)	32	17	49, 135, 174, 184	0
All	All	5670/5906 (96%)	0.10	198 (3%)	47	27	22, 60, 120, 184	0

The worst 5 of 198 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	458	ILE	7.6
1	E	307	HIS	6.6
1	E	285	SER	5.8
3	D	232	ARG	5.8
1	E	310	PHE	5.7

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
5	CA	B	4000	1/1	0.96	0.10	67,67,67,67	0
5	CA	E	4000	1/1	0.97	0.09	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.