



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:32 PM GMT

PDB ID : 4F5X  
Title : Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles  
Authors : Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.  
Deposited on : 2012-05-13  
Resolution : 5.00 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](mailto: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.

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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 : **FAILED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

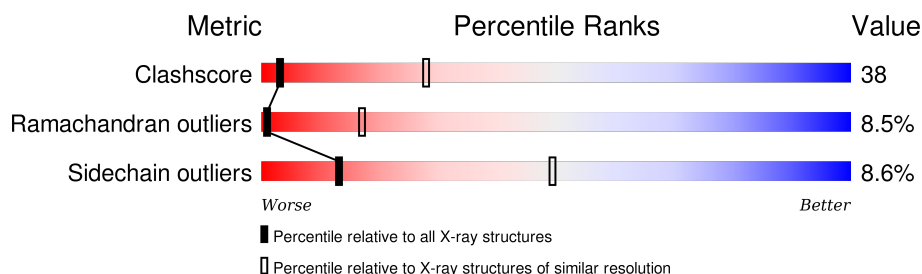
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.00 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	102246	1019 (6.22-3.66)
Ramachandran outliers	100387	1158 (6.22-3.60)
Sidechain outliers	100360	1136 (6.22-3.60)










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  $\geq 3$ , 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	
2	C	397	
2	D	397	
2	E	397	
2	F	397	
2	G	397	

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Mol	Chain	Length	Quality of chain
2	H	397	 60% 32% 7% .
2	I	397	 58% 33% 9%
2	J	397	 58% 34% 8% .
2	K	397	 59% 33% 8% .
2	L	397	 57% 35% 7% .
2	M	397	 58% 35% 6% .
2	N	397	 56% 34% 9% .
2	O	397	 57% 33% 9% .
3	W	1089	 40% 44% 5% 10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 62014 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 VP2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	975	Total	C	N	O	S	0	0	0
			7905	5081	1308	1482	34			

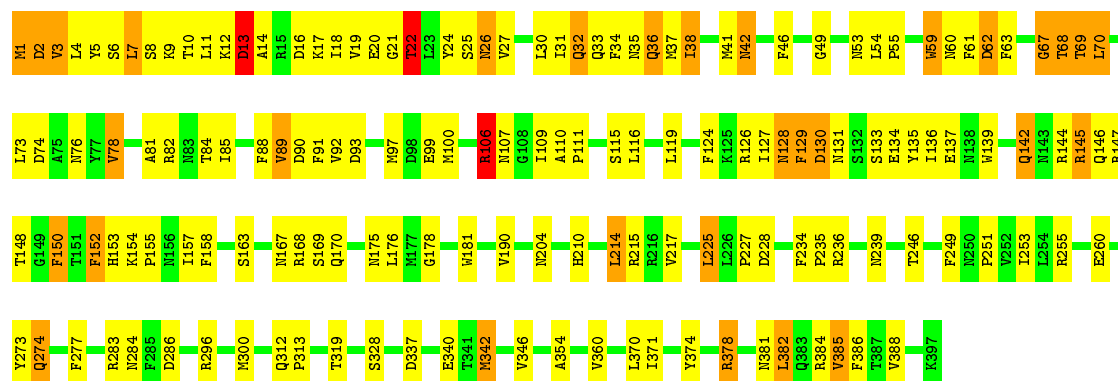
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		

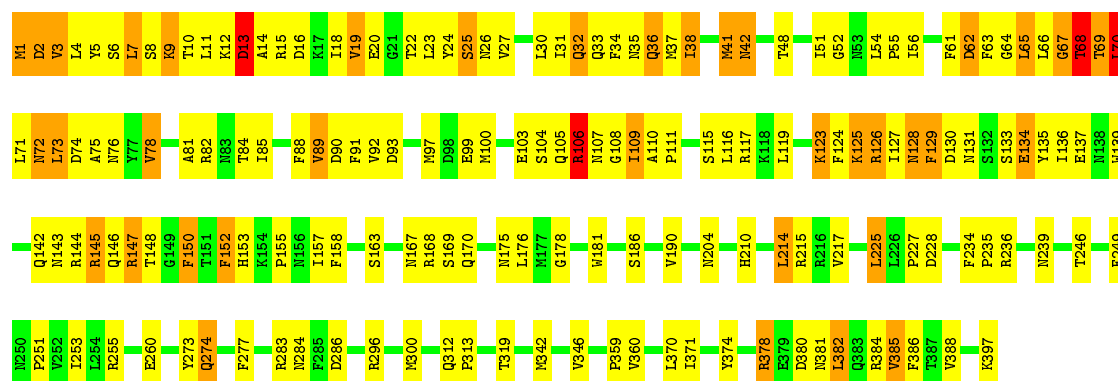


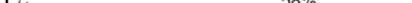
S696	D697	A758	V757	S821	S769	A706	S821
D697	A758	V757	A758	1622	S770	A707	1622
K698	L759	A759	A758	K824	S771	A708	K824
L759	A759	A759	A758	1699	I772	D709	1699
A700	A760	A760	A759	Y826	S773	A710	Y826
A701	A761	A761	A759	Y825	A774	A711	Y825
G702	A762	A762	A759	K827	I775	A712	K827
G703	A763	A763	A759	Q828	A776	A713	Q828
A703	A764	A764	A759	P830	A777	A714	P830
A704	A765	A765	A759	F833	A778	D715	F833
A705	A766	A766	A759	D834	A779	D716	D834
A706	A767	A767	A759	F835	A780	A717	F835
A707	A768	A768	A759	K836	A781	A718	K836
A708	A769	A769	A759	Y837	A782	A719	Y837
A709	A770	A770	A759	S838	A783	A720	S838
A710	A771	A771	A759	N839	A784	A721	N839
A711	A772	A772	A759	H840	A785	A722	H840
A712	A773	A773	A759	H841	A786	A723	H841
A713	A774	A774	A759	T843	A787	A724	T843
A714	A775	A775	A759	S844	A788	A725	S844
A715	A776	A776	A759	N845	A789	A726	N845
A716	A777	A777	A759	L846	A790	A727	L846
A717	A778	A778	A759	T847	A791	A728	T847
A718	A779	A779	A759	F848	A792	A729	F848
A719	A780	A780	A759	Y850	A793	A730	Y850
A720	A781	A781	A759	K851	A794	A731	K851
A721	A782	A782	A759	P852	A795	A732	P852
A722	A783	A783	A759	S853	A796	A733	S853
A723	A784	A784	A759	L854	A797	A734	L854
A724	A785	A785	A759	D855	A798	A735	D855
A725	A786	A786	A759	A856	A799	A736	A856
A726	A787	A787	A759	F857	A800	A737	F857
A727	A788	A788	A759	N858	A801	A738	N858
A728	A789	A789	A759	S859	A802	A739	S859
A729	A790	A790	A759	L860	A803	A740	L860
A730	A791	A791	A759	D861	A804	A741	D861
A731	A792	A792	A759	T862	A805	A742	T862
A732	A793	A793	A759	Y863	A806	A743	Y863
A733	A794	A794	A759	K864	A807	A744	K864
A734	A795	A795	A759	P865	A808	A745	P865
A735	A796	A796	A759	S866	A809	A746	S866
A736	A797	A797	A759	L867	A810	A747	L867
A737	A798	A798	A759	N868	A811	A748	N868
A738	A799	A799	A759	F869	A812	A749	F869
A739	A800	A800	A759	N870	A813	A750	N870
A740	A801	A801	A759	S871	A814	A751	S871
A741	A802	A802	A759	L872	A815	A752	L872
A742	A803	A803	A759	D873	A816	A753	D873
A743	A804	A804	A759	Y874	A817	A754	Y874
A744	A805	A805	A759	K875	A818	A755	K875
A745	A806	A806	A759	P876	A819	A756	P876
A746	A807	A807	A759	S877	A820	A757	S877
A747	A808	A808	A759	L878	A821	A758	L878
A748	A809	A809	A759	D879	A822	A759	D879
A749	A810	A810	A759	Y880	A823	A760	Y880
A750	A811	A811	A759	K881	A824	A761	K881
A751	A812	A812	A759	P882	A825	A762	P882
A752	A813	A813	A759	S883	A826	A763	S883
A753	A814	A814	A759	L884	A827	A764	L884
A754	A815	A815	A759	N885	A828	A765	N885
A755	A816	A816	A759	F886	A829	A766	F886
A756	A817	A817	A759	T887	A830	A767	T887
A757	A818	A818	A759	Y888	A831	A768	Y888
A758	A819	A819	A759	K889	A832	A769	K889
A759	A820	A820	A759	P890	A833	A770	P890
A760	A821	A821	A759	S891	A834	A771	S891
A761	A822	A822	A759	L892	A835	A772	L892
A762	A823	A823	A759	D893	A836	A773	D893
A763	A824	A824	A759	Y894	A837	A774	Y894
A764	A825	A825	A759	K895	A838	A775	K895
A765	A826	A826	A759	P896	A839	A776	P896
A766	A827	A827	A759	S897	A840	A777	S897
A767	A828	A828	A759	L898	A841	A778	L898
A768	A829	A829	A759	N899	A842	A779	N899
A769	A830	A830	A759	F900	A843	A780	F900
A770	A831	A831	A759	T901	A844	A781	T901
A771	A832	A832	A759	Y902	A845	A782	Y902
A772	A833	A833	A759	K903	A846	A783	K903
A773	A834	A834	A759	P904	A847	A784	P904
A774	A835	A835	A759	S905	A848	A785	S905
A775	A836	A836	A759	L906	A849	A786	L906
A776	A837	A837	A759	D907	A850	A787	D907
A777	A838	A838	A759	Y908	A851	A788	Y908
A778	A839	A839	A759	K909	A852	A789	K909
A779	A840	A840	A759	P910	A853	A790	P910
A780	A841	A841	A759	S911	A854	A791	S911
A781	A842	A842	A759	L912	A855	A792	L912
A782	A843	A843	A759	D913	A856	A793	D913
A783	A844	A844	A759	Y914	A857	A794	Y914
A784	A845	A845	A759	K915	A858	A795	K915
A785	A846	A846	A759	P916	A859	A796	P916
A786	A847	A847	A759	S917	A860	A797	S917
A787	A848	A848	A759	L918	A861	A798	L918
A788	A849	A849	A759	D919	A862	A799	D919
A789	A850	A850	A759	Y920	A863	A800	Y920
A790	A851	A851	A759	K921	A864	A801	K921
A791	A852	A852	A759	P922	A865	A802	P922
A792	A853	A853	A759	S923	A866	A803	S923
A793	A854	A854	A759	L924	A867	A804	L924
A794	A855	A855	A759	D925	A868	A805	D925
A795	A856	A856	A759	Y926	A869	A806	Y926
A796	A857	A857	A759	K927	A870	A807	K927
A797	A858	A858	A759	P928	A871	A808	P928
A798	A859	A859	A759	S929	A872	A809	S929
A799	A860	A860	A759	L930	A873	A810	L930
A800	A861	A861	A759	D931	A874	A811	D931
A801	A862	A862	A759	Y932	A875	A812	Y932
A802	A863	A863	A759	K933	A876	A813	K933
A803	A864	A864	A759	P934	A877	A814	P934
A804	A865	A865	A759	S935	A878	A815	S935
A805	A866	A866	A759	L936	A879	A816	L936
A806	A867	A867	A759	D937	A880	A817	D937
A807	A868	A868	A759	Y938	A881	A818	Y938
A808	A869	A869	A759	K939	A882	A819	K939
A809	A870	A870	A759	P940	A883	A820	P940
A810	A871	A871	A759	S941	A884	A821	S941
A811	A872	A872	A759	L942	A885	A822	L942
A812	A873	A873	A759	D943	A886	A823	D943
A813	A874	A874	A759	Y944	A887	A824	Y944
A814	A875	A875	A759	K945	A888	A825	K945
A815	A876	A876	A759	P946	A889	A826	P946
A816	A877	A877	A759	S947	A890	A827	S947
A817	A878	A878	A759	L948	A891	A828	L948
A818	A879	A879	A759	D949	A892	A829	D949
A819	A880	A880	A759	Y950	A893	A830	Y950
A820	A881	A881	A759	K951	A894	A831	K951
A821	A882	A882	A759	P952	A895	A832	P952
A822	A883	A883	A759	S953	A896	A833	S953
A823	A884	A884	A759	L954	A897	A834	L954
A824	A885	A885	A759	D955	A898	A835	D955
A825	A886	A886	A759	Y956	A899	A836	Y956
A826	A887	A887	A759	K957	A900	A837	K957
A827	A888	A888	A759	P958	A901	A838	P958
A828	A889	A889	A759	S959	A902	A839	S959
A829	A890	A890	A759	L960	A903	A840	L960
A830	A891	A891	A759	D961	A904	A841	D961
A831	A892	A892	A759	Y962	A905	A842	Y962
A832	A893	A893	A759	K963	A906	A843	K963
A833	A894	A894	A759	P964	A907	A844	P964
A834	A895	A895	A759	S965	A908	A845	S965
A835	A896	A896	A759	L966	A909	A846	L966
A836	A897	A897	A759	D967	A910	A847	D967
A837	A898	A898	A759	Y968	A911	A848	Y968
A838	A899	A899	A759	K969	A912	A849	K969
A839	A900	A900	A759	P970	A913	A850	P970
A840	A901	A901	A759	S971	A914	A851	S971
A841	A902	A902	A759	L972	A915	A852	L972
A842	A903	A903	A759	D973	A916	A853	D973
A843	A904	A904	A759	Y974	A917	A854	Y974
A844	A905	A905	A759	K975	A918	A855	K975
A845	A906	A906	A759	P976	A919	A856	P976
A846	A907	A907	A759	S977	A920	A857	S977
A847	A908	A908	A759	L978	A921	A858	L978
A848	A909	A909	A759	D979	A922	A859	D979
A849	A910	A910	A759	Y980	A923	A860	Y980
A850	A911	A911	A759	K981	A924	A861	K981
A851	A912	A912	A759	P982	A925	A862	P982
A852	A913	A913	A759	S983	A926	A863	S983
A853	A914	A914	A759	L984	A927	A864	L984
A854	A915	A915	A759	D985	A928	A865	D985
A855	A916	A916	A759	Y986	A929	A866	Y986
A856	A917	A917	A759	K987	A930	A867	K987
A857	A918	A918	A759	P988	A931	A868	P988
A858	A919	A919	A759	S989	A932	A869	S989
A859	A920	A920	A759	L990	A933	A870	L990
A860	A921	A921	A759	D991	A934	A871	D991
A861	A922	A922	A759	Y992	A935	A872	Y992
A862	A923	A923	A759	K993	A936	A873	K993
A863	A924	A924	A759	P994	A937	A874	P994
A864	A925	A925	A759	S995	A938	A875	S995
A865	A926	A926	A759	L996	A939	A876	L996
A866	A927	A927	A759	D997	A940	A877	D997
A867	A928	A928	A759	Y998	A941	A878	Y998
A868	A929	A929	A759	K999	A942	A879	K999
A869	A930	A930	A759	P1000	A943	A880	P1000
A870	A931	A931	A759	S1001	A944	A881	S1001
A871	A932	A932	A759	L1002	A		

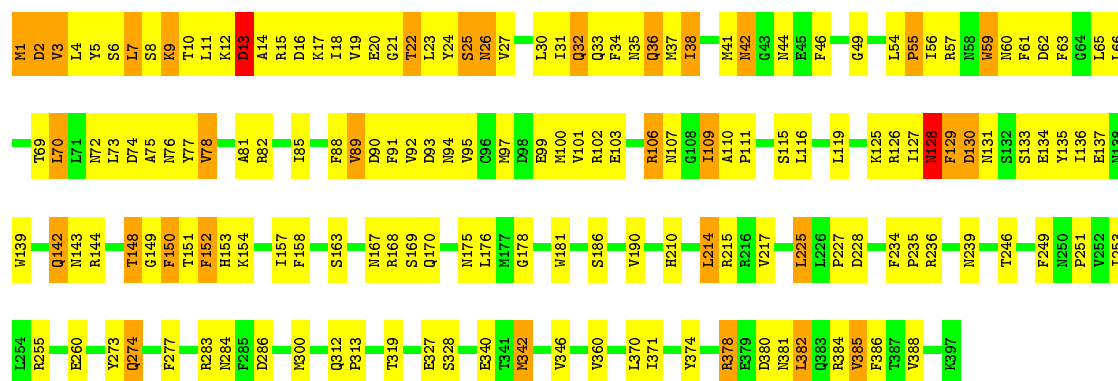
Chain C:  60% 31% 8%

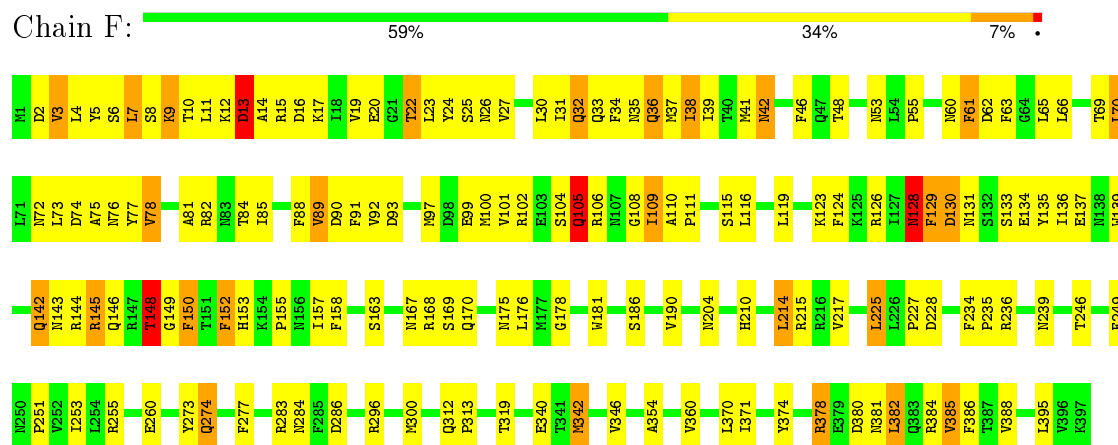


Chain D:  57% 32% 9%

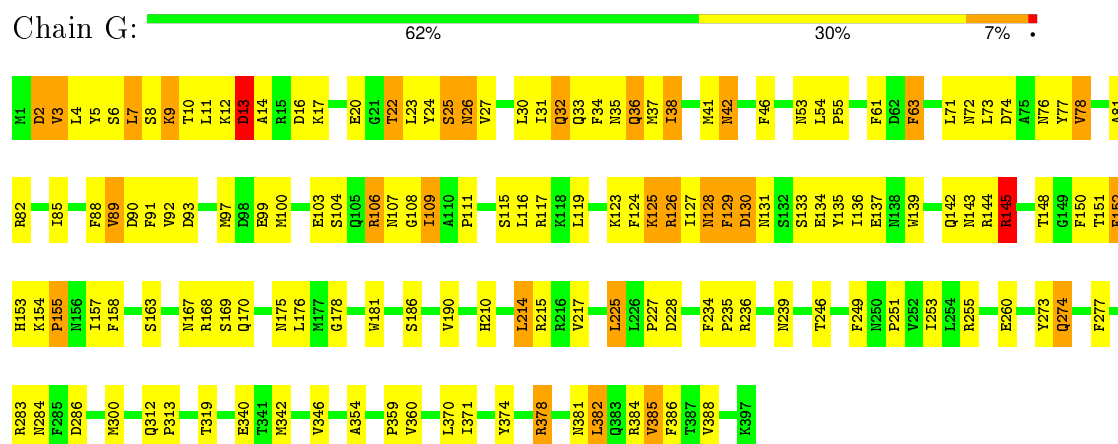


Chain E:  58% 33% 8%

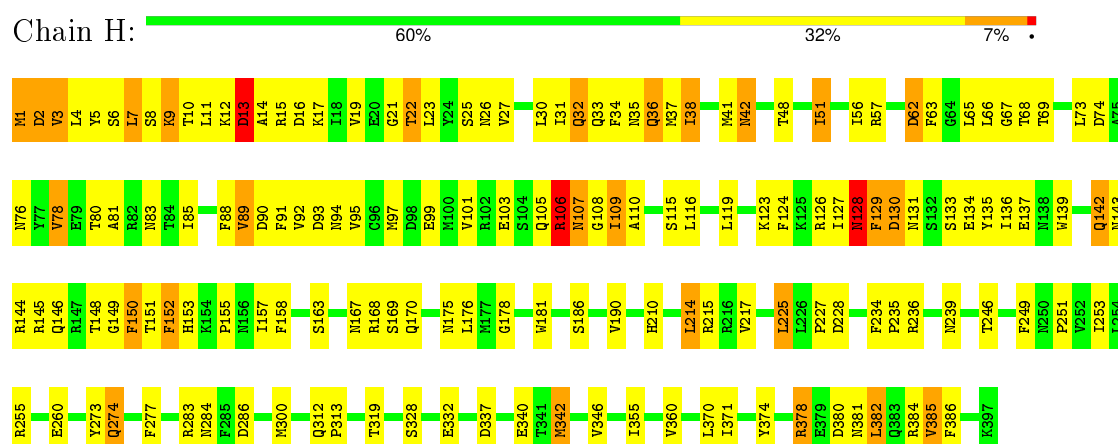




• Molecule 2: Intermediate capsid protein VP6

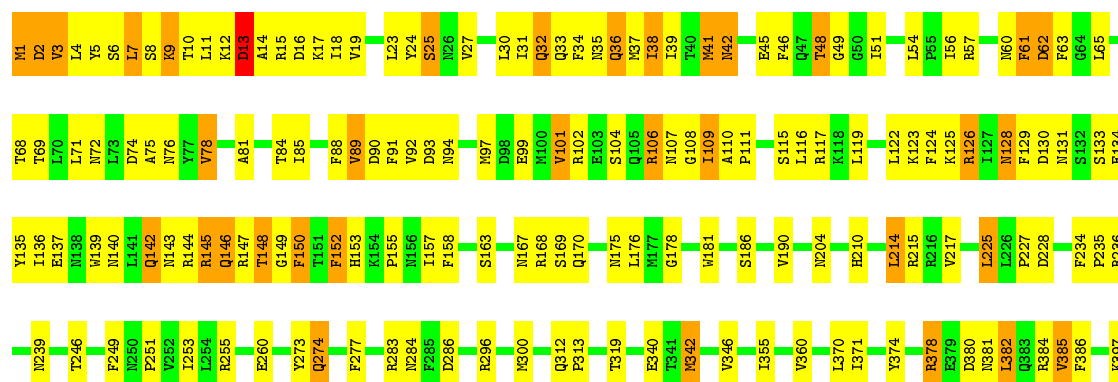


• Molecule 2: Intermediate capsid protein VP6

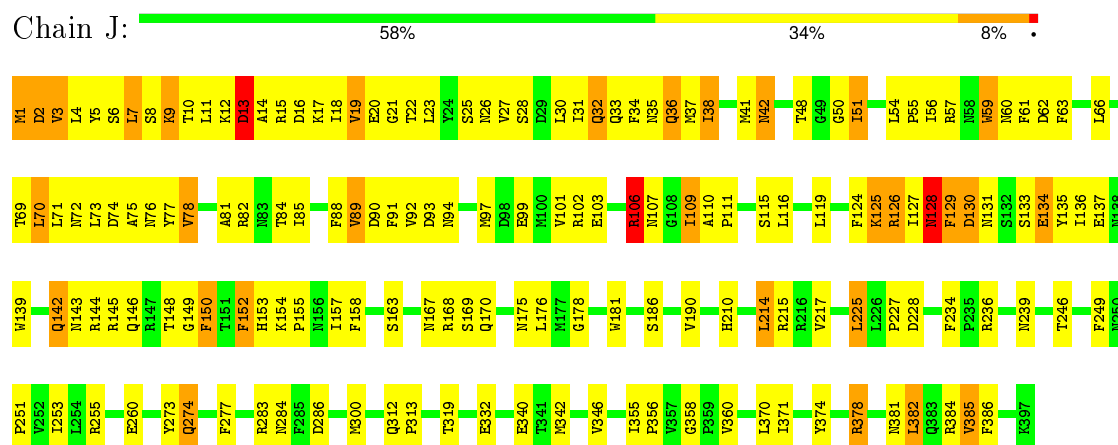


• Molecule 2: Intermediate capsid protein VP6

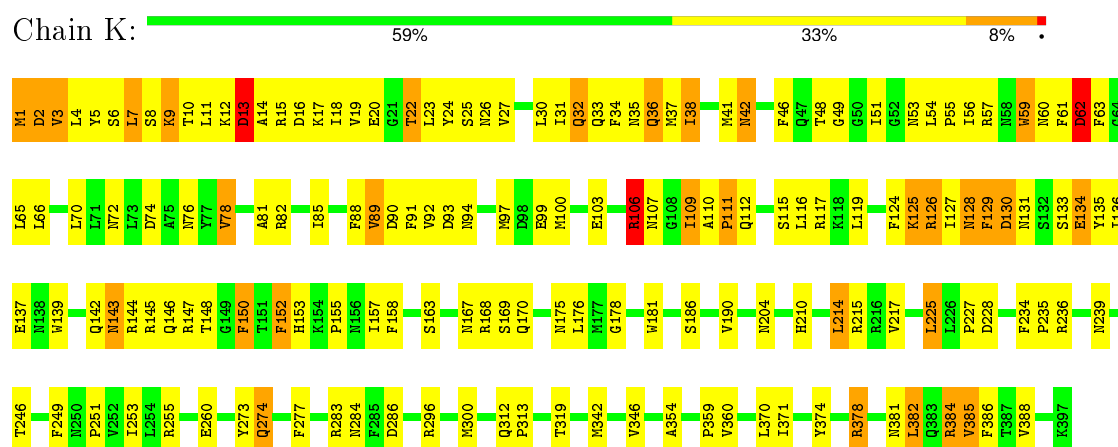




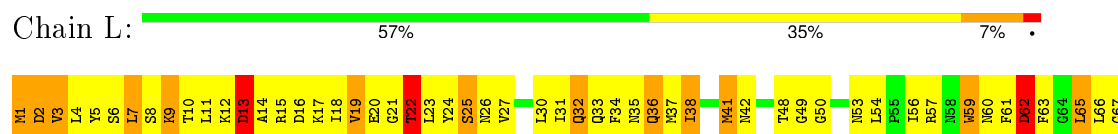
• Molecule 2: Intermediate capsid protein VP6

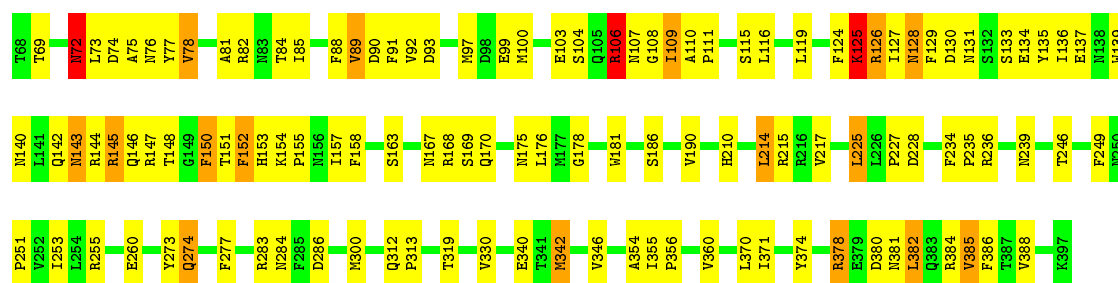


• Molecule 2: Intermediate capsid protein VP6



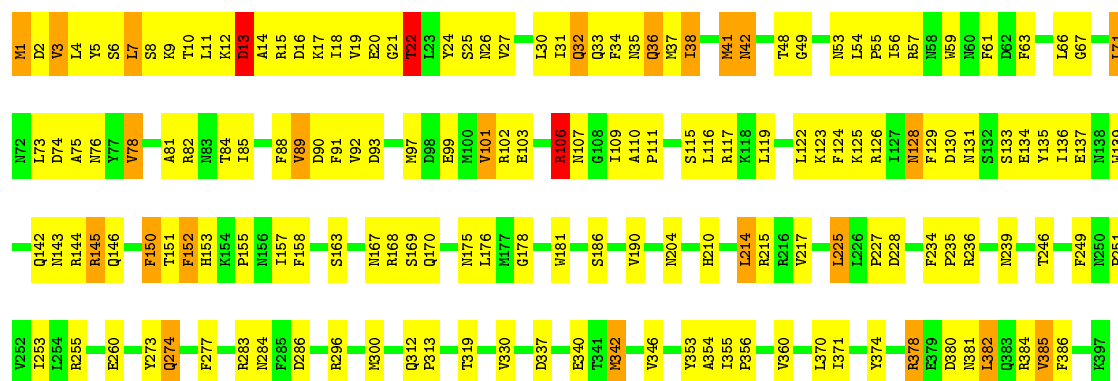
• Molecule 2: Intermediate capsid protein VP6





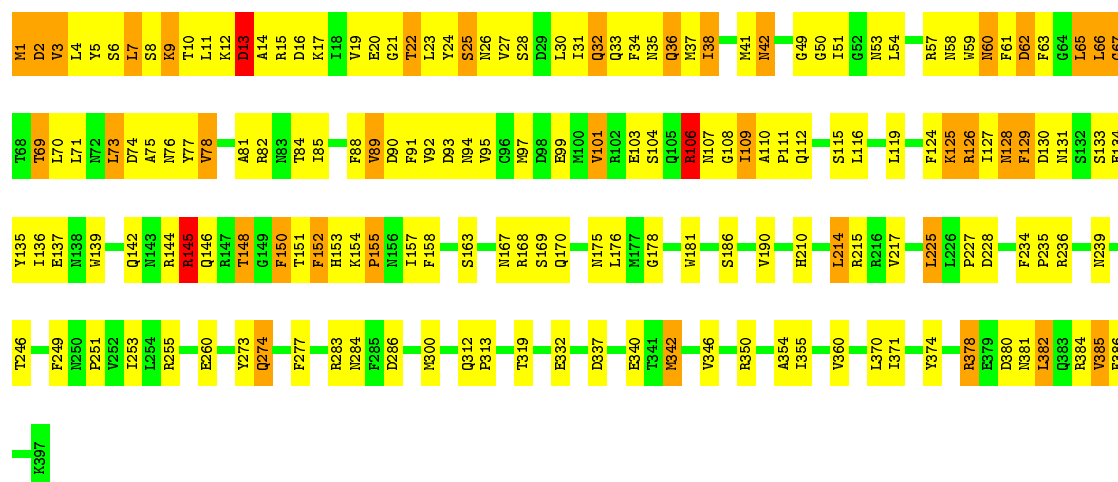
• Molecule 2: Intermediate capsid protein VP6

Chain M: 58% 35% 6% .



• Molecule 2: Intermediate capsid protein VP6

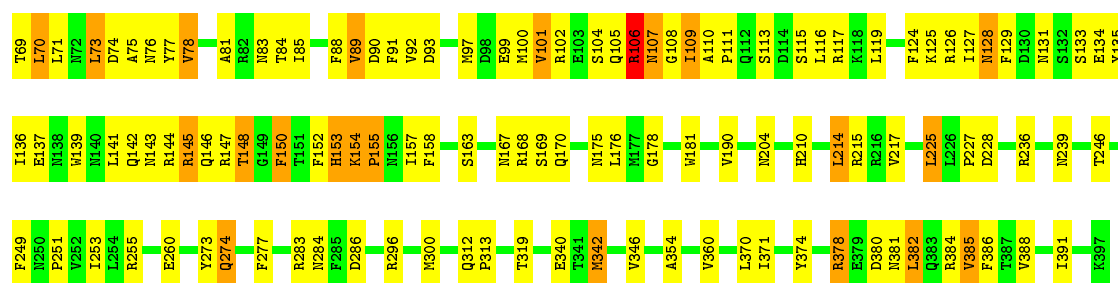
Chain N: 56% 34% 9% .



• Molecule 2: Intermediate capsid protein VP6

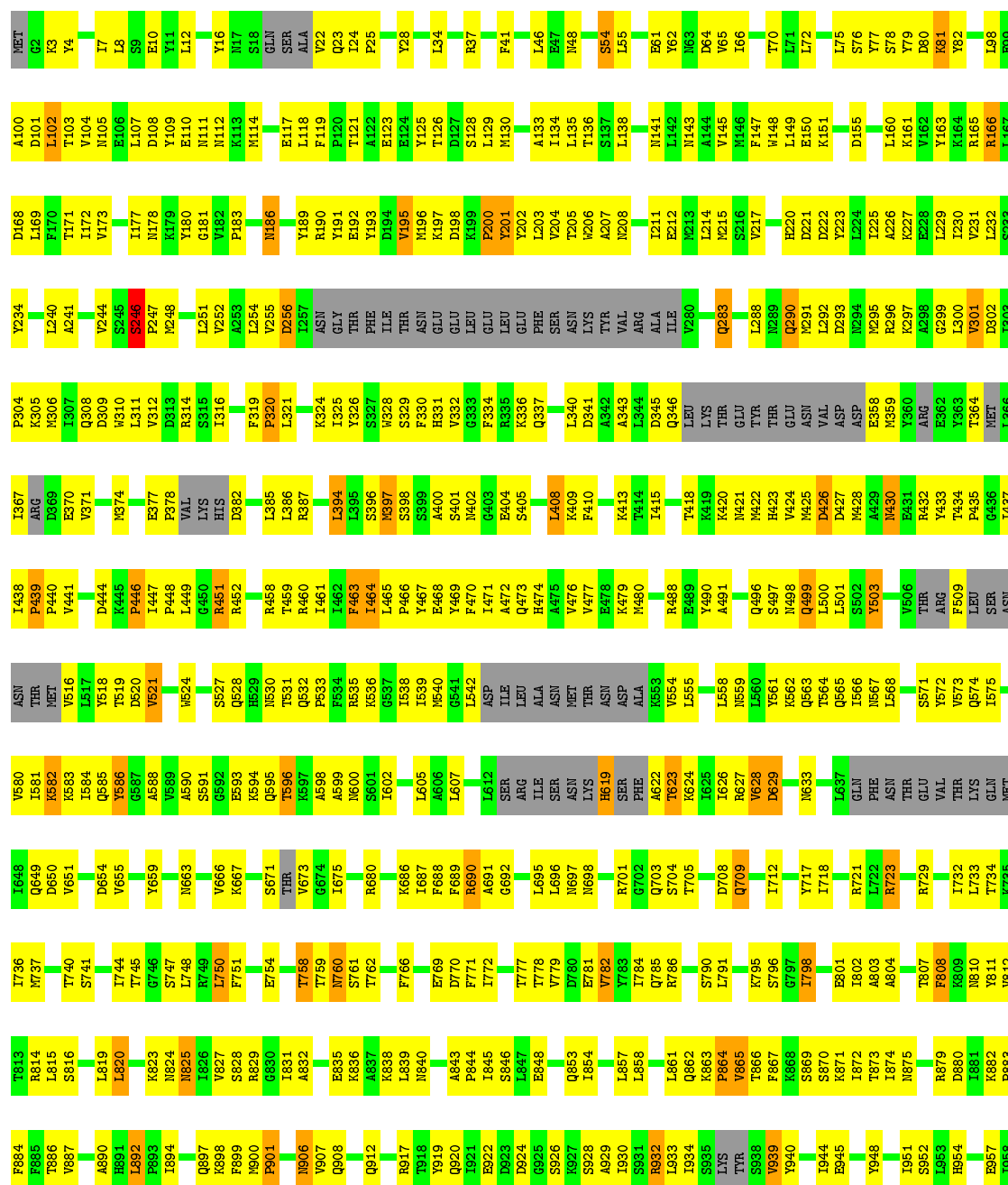
Chain O: 57% 33% 9% .





• Molecule 3: RNA-directed RNA polymerase

Chain W: 40% 44% 5% 10%



LYS	ILE	PRO	ALA	VAL	THR	F1031	H1034	A1037	I1042	M1043	K1047	N1048	G1049	S1050	W1051	I1052	S1053	L1054	Y1058	P1059	M1063	K1068	K1069	M1070	W1071	M1072	I1073	T1074	R1077	S1078	P1079	Y1080	T1081	M1082	A1083	M1084	F1085	F1086	GLN	GLU	PRO												
GLN	LEU	Y961	I962	ILE	S964	L965	G966	PRO	LYS	ILE	ASP	ALA	ASP	THR	TYR	VAL	GLY	SER	LYS	ILE	Y981	S982	ARG	D984	R985	Y986	R987	I988	S991	Y992	I996	I999	M1000	Y1001	G1002	C1003	Y1004	Q1005	L1006	F1009	M1010	D1013	L1014	GLU	K1016	L1017	I1018	R1019	ILE	PRO	PHE	LYS	GLY

## 4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 5.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-5.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.293 , 0.296	Depositor
Wilson B-factor (Å <sup>2</sup> )	167.1	Xtriage
Anisotropy	0.043	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 2393850 reflections (0.000%)	Xtriage
Total number of atoms	62014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/6491	0.84	9/8806 (0.1%)
1	B	0.50	0/6745	0.82	10/9149 (0.1%)
2	C	0.51	0/3232	0.78	5/4397 (0.1%)
2	D	0.51	0/3232	0.78	5/4397 (0.1%)
2	E	0.51	0/3232	0.77	5/4397 (0.1%)
2	F	0.50	0/3232	0.76	5/4397 (0.1%)
2	G	0.50	0/3232	0.77	5/4397 (0.1%)
2	H	0.50	0/3232	0.76	5/4397 (0.1%)
2	I	0.50	0/3232	0.77	5/4397 (0.1%)
2	J	0.51	0/3232	0.78	5/4397 (0.1%)
2	K	0.51	0/3232	0.77	5/4397 (0.1%)
2	L	0.51	0/3232	0.77	5/4397 (0.1%)
2	M	0.51	0/3232	0.77	5/4397 (0.1%)
2	N	0.51	0/3232	0.77	5/4397 (0.1%)
2	O	0.52	0/3232	0.79	7/4397 (0.2%)
3	W	0.41	0/8045	0.62	3/10847 (0.0%)
All	All	0.49	0/63297	0.77	89/85963 (0.1%)

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	A	0	1

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	10.70	127.42	121.00
1	A	273	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	273	TYR	CA-CB-CG	9.85	132.12	113.40
1	B	273	TYR	CB-CG-CD1	9.85	126.91	121.00
1	B	273	TYR	CB-CG-CD2	-9.21	115.48	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

## 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	6374	0	6394	1006	0
1	B	6624	0	6652	1133	0
2	C	3162	0	3101	170	0
2	D	3162	0	3101	179	0
2	E	3162	0	3101	164	0
2	F	3162	0	3101	160	0
2	G	3162	0	3101	149	0
2	H	3162	0	3101	175	0
2	I	3162	0	3101	215	0
2	J	3162	0	3101	187	0
2	K	3162	0	3101	166	0
2	L	3162	0	3101	178	0
2	M	3162	0	3101	173	0
2	N	3162	0	3101	191	0
2	O	3162	0	3101	163	0
3	W	7905	0	7966	543	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	O	1	0	0	0	0
All	All	62014	0	61325	4691	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 38.

The worst 5 of 4691 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:75:VAL:HG22	3:W:673:VAL:CG1	1.63	1.28
1:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:B:75:VAL:CG2	3:W:673:VAL:HG12	1.72	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13

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	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	3
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	3
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	2	27
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	20
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	27
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	2	26
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	27
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2	28
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	2	26
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2	28
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	2	26
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2	30
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	22
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	19
3	W	933/1089 (86%)	807 (86%)	93 (10%)	33 (4%)	4	40
All	All	7655/8010 (96%)	5858 (76%)	1147 (15%)	650 (8%)	1	17

5 of 650 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	ALA

### 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	715/809 (88%)	603 (84%)	112 (16%)	3	23
1	B	744/809 (92%)	635 (85%)	109 (15%)	4	25
2	C	350/350 (100%)	325 (93%)	25 (7%)	18	57
2	D	350/350 (100%)	322 (92%)	28 (8%)	15	52
2	E	350/350 (100%)	325 (93%)	25 (7%)	18	57
2	F	350/350 (100%)	327 (93%)	23 (7%)	21	59
2	G	350/350 (100%)	327 (93%)	23 (7%)	21	59
2	H	350/350 (100%)	329 (94%)	21 (6%)	24	62
2	I	350/350 (100%)	327 (93%)	23 (7%)	21	59
2	J	350/350 (100%)	327 (93%)	23 (7%)	21	59
2	K	350/350 (100%)	327 (93%)	23 (7%)	21	59
2	L	350/350 (100%)	321 (92%)	29 (8%)	14	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	350/350 (100%)	325 (93%)	25 (7%)	18	57
2	N	350/350 (100%)	324 (93%)	26 (7%)	17	55
2	O	350/350 (100%)	329 (94%)	21 (6%)	24	62
3	W	885/990 (89%)	828 (94%)	57 (6%)	22	60
All	All	6894/7158 (96%)	6301 (91%)	593 (9%)	13	49

5 of 593 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	284	ASN
2	G	143	ASN
3	W	198	ASP
2	E	13	ASP
2	F	60	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 253 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	53	ASN
2	I	131	ASN
3	W	499	GLN
2	G	142	GLN
2	H	128	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.