



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 09:17 PM EDT

PDB ID : 3SHF / pdb_00003shf
Title : Crystal structure of the R265S mutant of full-length murine Apaf-1
Authors : Eschenburg, S.; Reubold, T.F.
Deposited on : 2011-06-16
Resolution : 3.55 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

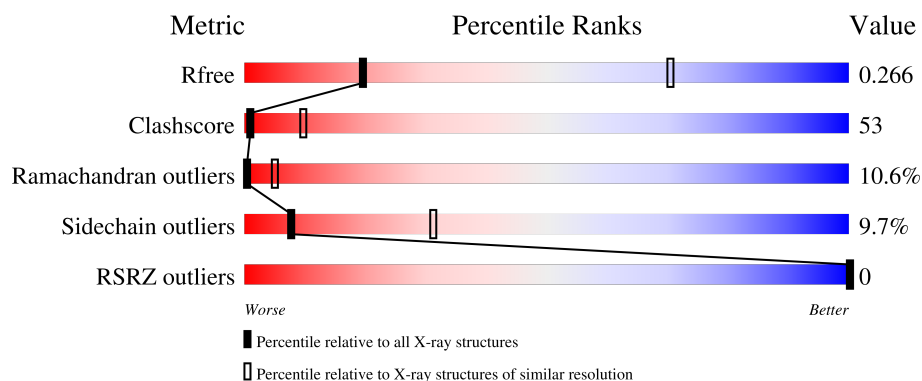
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

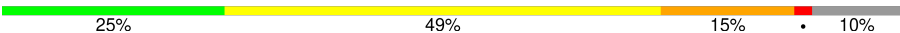
The reported resolution of this entry is 3.55 Å.

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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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	A	1256	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9122 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.

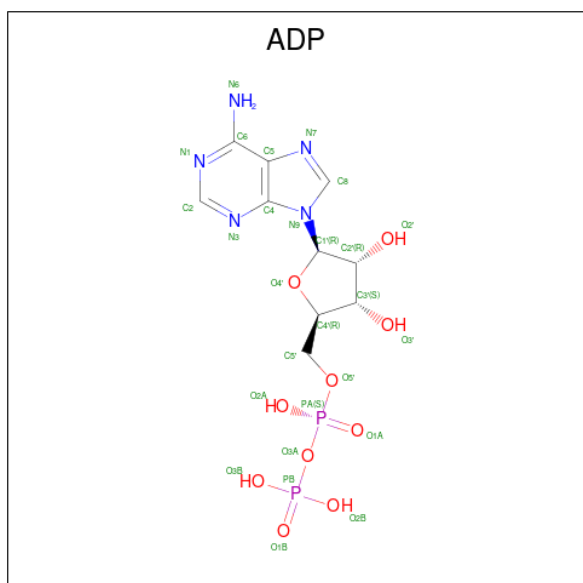
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1133	9010	5712	1551	1692	55	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

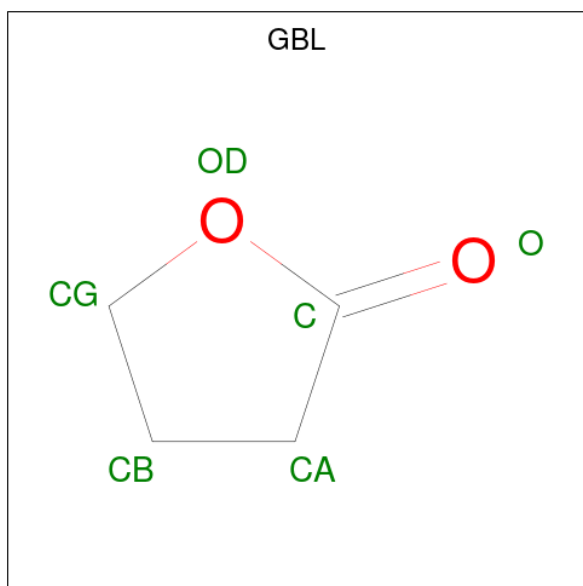
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A2RRK8
A	-5	ALA	-	expression tag	UNP A2RRK8
A	-4	MET	-	expression tag	UNP A2RRK8
A	-3	ASP	-	expression tag	UNP A2RRK8
A	-2	PRO	-	expression tag	UNP A2RRK8
A	-1	GLU	-	expression tag	UNP A2RRK8
A	0	PHE	-	expression tag	UNP A2RRK8
A	265	SER	ARG	engineered mutation	UNP A2RRK8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GAMMA-BUTYROLACTONE (CCD ID: GBL) (formula: $C_4H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		

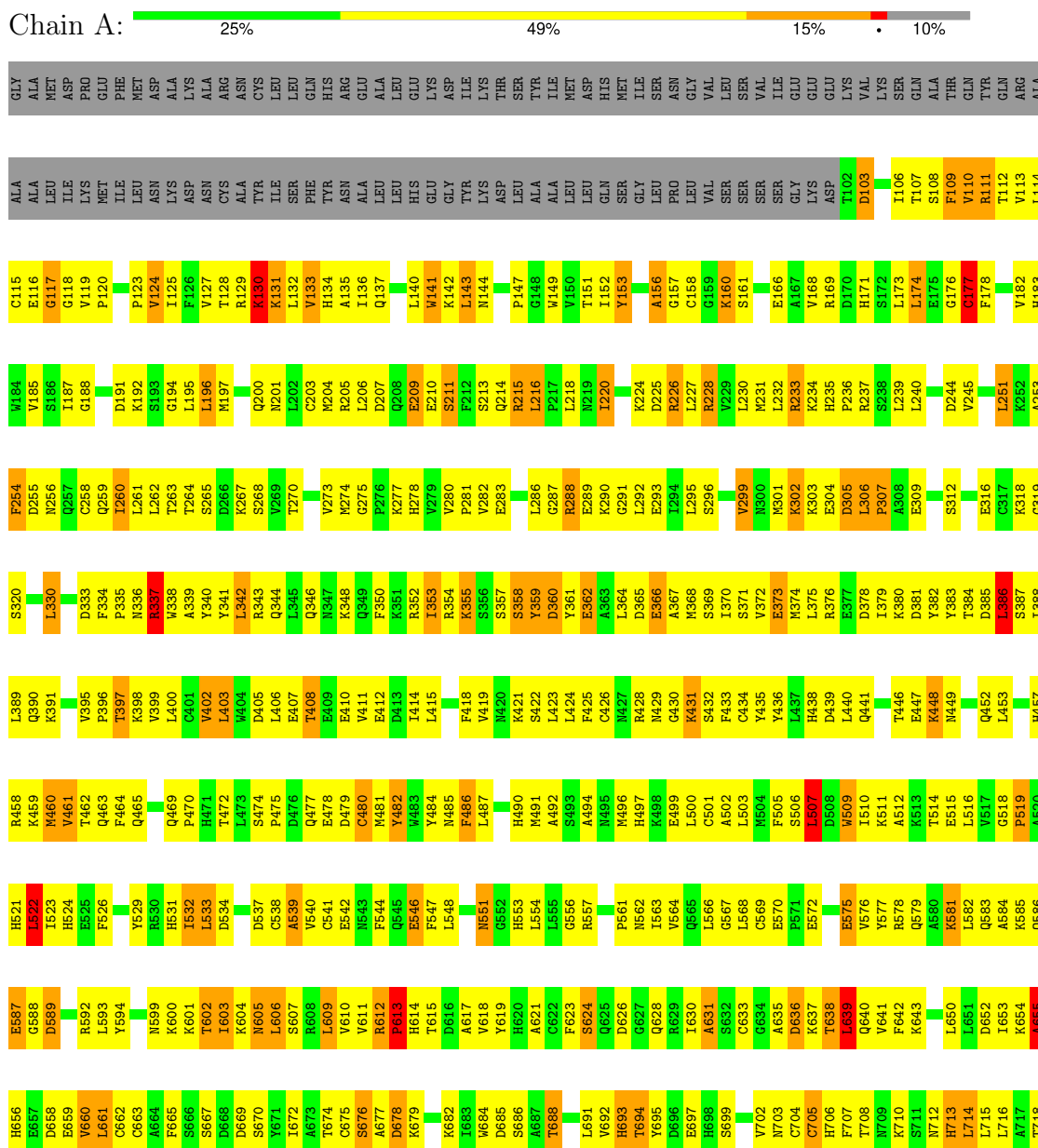
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		

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: Apoptotic peptidase activating factor 1



L1242	L1243	Y1244	I1245	Q1246	V1247	L1248	E1249	ALA	THR	H1177	G1178	G1179	H1180	V1181	T1182	D1183	V1184	C1185	F1186	S1187	P1188	D1189	S1190	K1191	T1192	L1193	V1194	K1201	W1202	W1203	M1204	V1205	A1206	T1207	S1210	S1211	Q1212	T1213	F1214	M1217	G1218	T1219	N1220	L1221	K1222	K1223	I1224	H1225	V1226	S1227	P1228	D1229	F1230	R1231	T1232	Y1233	V1234	T1235	V1236	D1237	N1238	L1239	G1240	I1241	D1115	L1116	L1117	S1118	P1119	L1120	H1121	E1122	L1123	K1124	C1125	H1126	N1127	G1128	C1129	V1130	R1131	C1132	S1133	A1134	F1135	S1136	L1137	D1138	G1139	I1140	L1141	A1143	T1144	G1145	D1146	D1147	N1148	E1150	I1151	R1152	I1153	W1154	N1155	V1156	S1157	D1158	G1159	Q1160	L1161	H1162	S1164	C1165	A1166	P1167	I1168	S1169	VAL	GLU	GLU	GLY	THR	D11052	L1053	Q1054	R1057	L1058	L1059	S1060	W1061	S1062	F1063	D1064	R1065	T1066	V1067	K1068	V1069	W1070	M1071	V1072	I1073	T1074	G1075	R1076	I1077	E1078	R1079	D1080	F1081	T1082	G1083	H1084	T1087	V1088	L1089	S1090	C1091	A1092	I1093	S1094	S1095	D1096	A1097	T1098	S1101	S1102	T1103	S1104	A1105	D1106	K1107	T1108	A1109	K1110	I1111	W1112	S1113	F1114	D982	G983	A984	I985	K986	I987	T988	E989	L990	P991	N992	N993	R994	V995	S998	G1001	H1002	K1003	V1006	R1007	H1008	I1009	Q1010	F1011	T1012	A1013	D1014	G1015	K1016	T1017	L1018	I1019	E1023	D1024	S1025	V1026	I1027	Q1028	V1029	W1030	M1031	W1032	T1034	Q1041	A1042	H1043	Q1044	E1045	T1046	V1047	K1048	D1049	F1050	R1051	A919	I920	V921	L922	K923	Q924	E925	I926	D927	S928	F929	Y930	Q931	E932	N933	E934	L938	A939	V940	D941	N942	I943	R944	G945	L946	Q947	L948	I949	A950	S951	K952	T953	G954	Q955	I956	D957	Y958	L959	P960	E961	A962	L963	V964	C967	C968	L969	S970	P971	H972	L973	E974	Y975	V976	A977	F978	G979	D980	R1051	D847	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q844	T843	R842	S841	E810	H840	D839	Q838	T837	H836	I835	L832	L831	G830	S829	T828	A827	S826	L825	P824	L823	V821	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T778	Y845	Q84
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.88Å 111.82Å 244.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.55 20.00 – 3.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.55) 98.9 (20.00-3.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.305 0.212 , 0.266	Depositor DCC
R_{free} test set	8050 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GBL, ADP

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	0.54	0/9206	1.05	69/12465 (0.6%)

There are no bond length outliers.

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	MET	N-CA-C	-10.61	95.71	110.35
1	A	871	SER	N-CA-C	-9.33	101.91	113.38
1	A	1113	SER	N-CA-C	8.99	124.16	111.30
1	A	109	PHE	N-CA-C	-7.91	101.30	112.13
1	A	429	ASN	N-CA-C	-7.73	103.18	114.39

There are no chirality outliers.

There are no planarity outliers.

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	A	9010	0	8875	954	0
2	A	27	0	12	3	0
3	A	12	0	12	1	0
4	A	73	0	0	3	0
All	All	9122	0	8899	954	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 954 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:A:216:LEU:HD12	1:A:216:LEU:H	1.13	1.08
1:A:182:VAL:HG12	1:A:239:LEU:HB3	1.36	1.06
1:A:1108:THR:HG21	1:A:1124:LYS:HA	1.35	1.05
1:A:288:ARG:HE	1:A:288:ARG:N	1.58	1.00
1:A:785:ARG:HG3	1:A:785:ARG:HH11	1.28	0.97

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	1127/1256 (90%)	765 (68%)	242 (22%)	120 (11%)	0 5

5 of 120 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	174	LEU
1	A	177	CYS
1	A	253	ALA
1	A	337	ARG

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	A	1005/1109 (91%)	908 (90%)	97 (10%)	8	31

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	866	LEU
1	A	992	ASN
1	A	871	SER
1	A	946	LEU
1	A	1019	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	942	ASN
1	A	1031	ASN
1	A	955	GLN
1	A	993	ASN
1	A	1127	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands 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	$\# Z > 2$
2	ADP	A	1250	-	28,29,29	1.85	6 (21%)	43,45,45	1.94	10 (23%)
3	GBL	A	1252	-	6,6,6	0.73	0	7,7,7	0.78	0
3	GBL	A	1251	-	6,6,6	1.03	0	7,7,7	0.79	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
2	ADP	A	1250	-	-	0/16/32/32	0/3/3/3
3	GBL	A	1252	-	-	-	0/1/1/1
3	GBL	A	1251	-	-	-	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ADP	PA-O3A	6.73	1.66	1.59
2	A	1250	ADP	C6-N6	2.84	1.41	1.34
2	A	1250	ADP	C5-C4	2.60	1.43	1.39
2	A	1250	ADP	PB-O3B	2.47	1.64	1.54
2	A	1250	ADP	O4'-C1'	2.13	1.46	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ADP	C5-C4-N3	-5.38	119.31	126.72
2	A	1250	ADP	N3-C2-N1	-4.56	121.67	128.58
2	A	1250	ADP	N3-C4-N9	4.47	134.77	127.17
2	A	1250	ADP	C2-N3-C4	4.04	121.69	111.83
2	A	1250	ADP	C5-N7-C8	3.69	109.25	103.45

There are no chirality outliers.

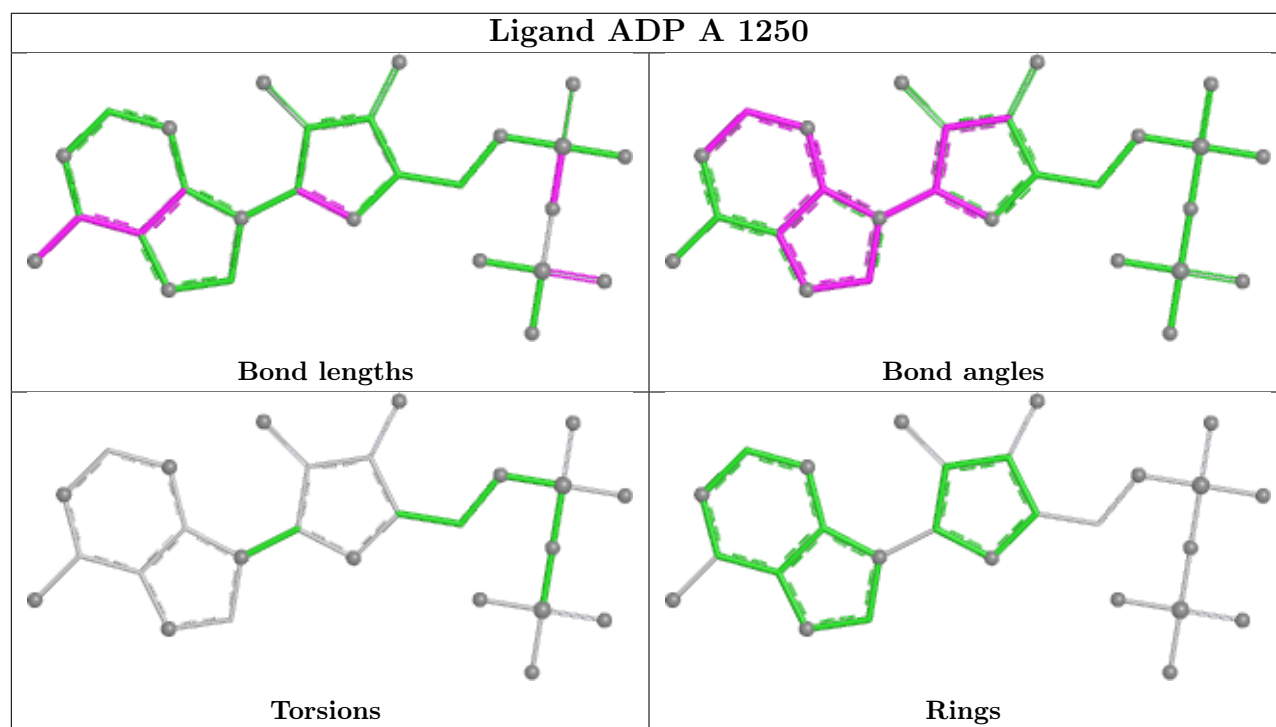
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1250	ADP	3	0
3	A	1251	GBL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1133/1256 (90%)	-0.41	0 100 100	74, 106, 140, 175	0

There are no RSRZ outliers to report.

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](#)

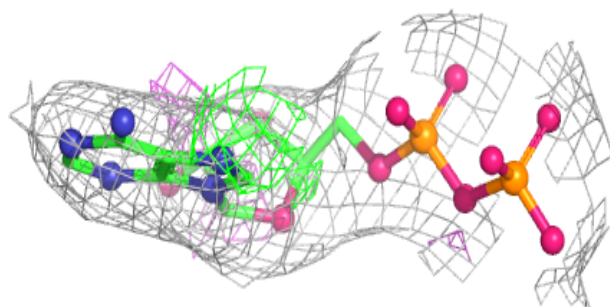
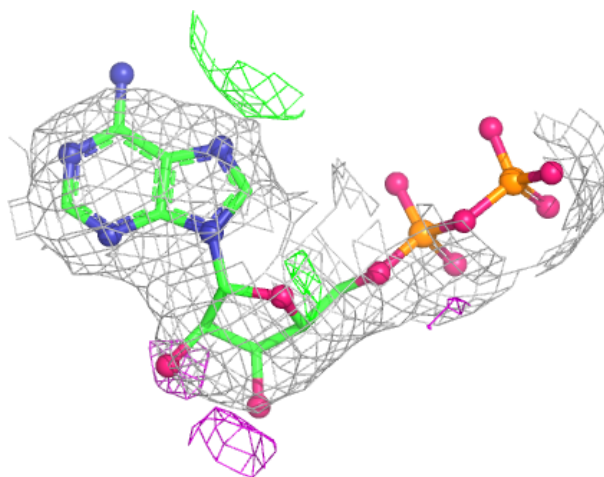
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	1250	27/27	0.95	0.08	81,86,90,90	0
3	GBL	A	1251	6/6	0.95	0.10	91,92,92,93	0
3	GBL	A	1252	6/6	0.96	0.12	100,101,102,103	0

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

Electron density around ADP A 1250:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.