



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 11:19 pm BST

PDB ID : 3SHF
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

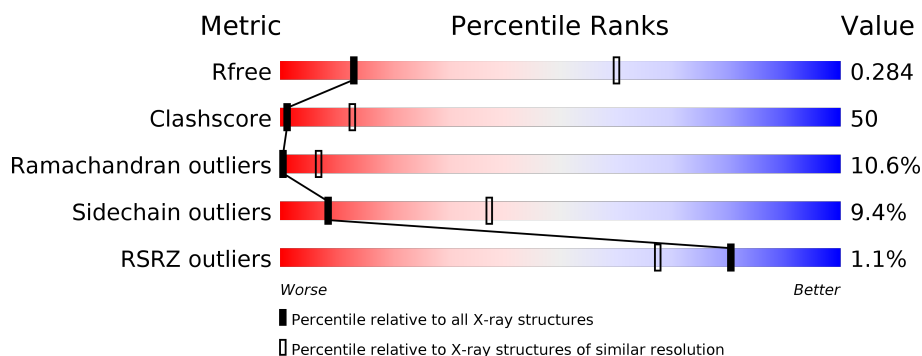
1 Overall quality at a glance

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}	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div> <div></div> <div>29%</div> <div>48%</div> <div>12%</div> <div>10%</div> </div> </div>

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.

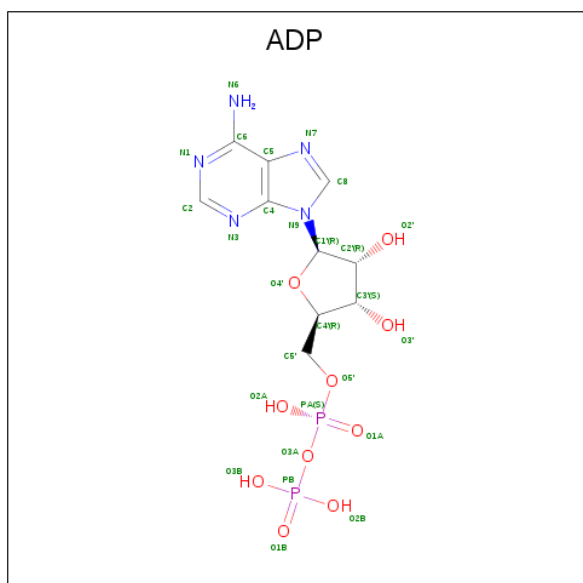
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

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:

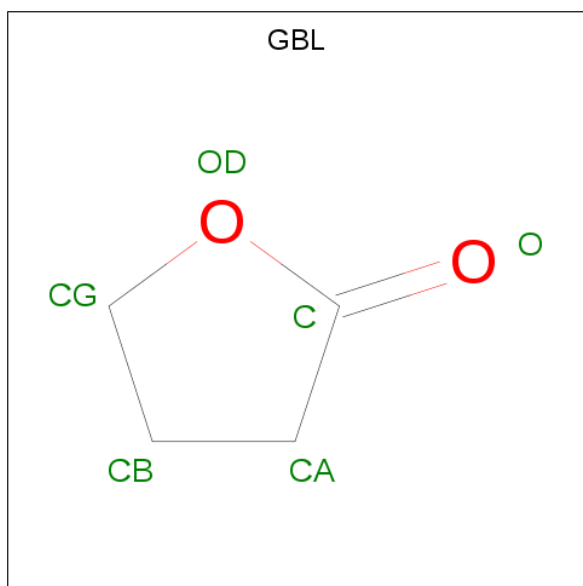
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP A2RRK8
A	-5	ALA	-	EXPRESSION TAG	UNP A2RRK8
A	-4	MET	-	EXPRESSION TAG	UNP A2RRK8
A	-3	ASP	-	EXPRESSION TAG	UNP A2RRK8
A	-2	PRO	-	EXPRESSION TAG	UNP A2RRK8
A	-1	GLU	-	EXPRESSION TAG	UNP A2RRK8
A	0	PHE	-	EXPRESSION TAG	UNP A2RRK8
A	265	SER	ARG	ENGINEERED MUTATION	UNP A2RRK8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: 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 (three-letter code: 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		

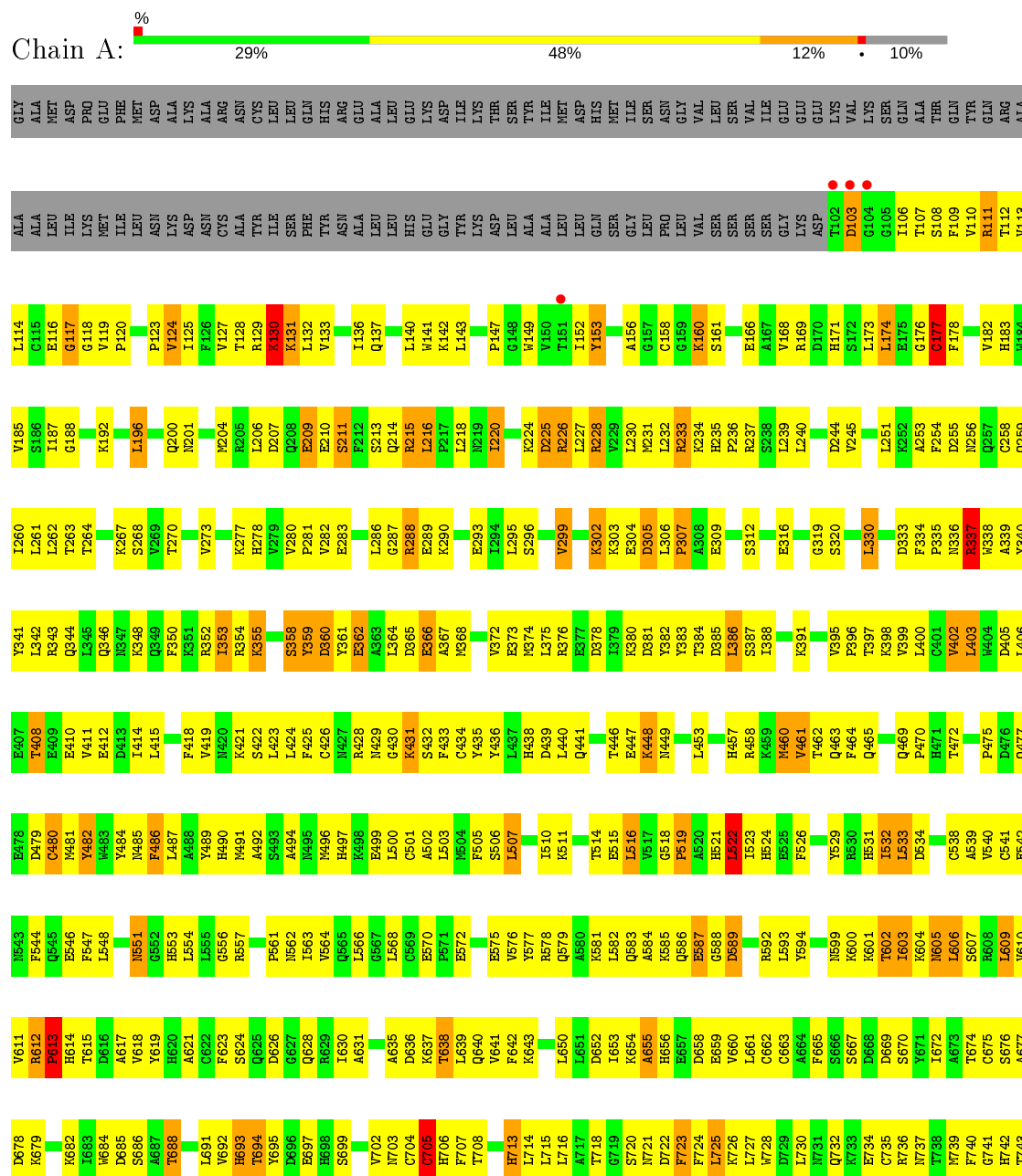
- Molecule 4 is water.

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 and DNA 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



T1207	L1142	D1080	F1011	Q947	B879	G810	N744
S1210	A1143	F1081	T1012	C968	G880	D811	S745
S1211	T1144	T1082	A1013	L948	H881	R812	V746
Q1212	G1145	C1083	D1014	I949	L882	R813	N747
T1213	D1146	H1084	G1015	Q950	G951	R814	H748
F1214	D1147	T1087	K1016	K952	K834	R815	C749
	N1148	V1088	T1017	T953	V888	R750	R750
	G1149	V1086	L1018	G954	V888	F751	F751
	I1150	S1089	I1019	Q955	M889	S752	S752
	I1151	S1090		I956	F890	P753	P753
	R1152	C1091	E1023	D957	S891	L822	D754
	I1153	A1092	D1024	Y958	P892	L823	D755
	H1154	I1083	S1025	L959	D893	F824	E756
	N1155	S1094	V1026	P960	G894	D825	L757
	V1156	S1095	I1027	E961	S895	I826	L758
	H1225	D1096	Q1028	A962	S896	H827	A759
	V1226	A1097	V1029	Q963	F897	T828	S760
	D1158	T1098	W1030	V964	L898	S829	C761
	G1159		W1031	T899	G830	S762	S762
	Q1160		W1032	C967	L831	A763	A763
	L1161	S1101	Q1033	C968	L832	D764	D764
	L1162	S1102		L969	A833	L767	L767
	H1163	T1103	Q1041	S970	E834	R768	R768
	S1164	S1104	A1042	P971	T905	L769	L769
	C1165	A1105	H1043	H972	I906	W770	W770
	A1166	D1106	Q1044	L973	A907	D771	D771
	P1167	K1107	E1045	E974	V908	W772	W772
	I1168	T1108	T1046	Y975	W909	R773	R773
	S1169	A1109	V1047	V976	E910	S774	S774
	VAL	K1110	K1048	A977	K913	A775	A775
	GLU	I1111	D1049	F978	Q844	R778	R778
	GLY	W1112	F1050	G979	Y845	V783	V783
	THR	S1113	A1051	D980	C846	K784	K784
	ALA	D1115	L1052	E981	D847	R785	R785
	THR	L1116	L1053	D982	F849	F786	F786
	H1177	L1117	Q1054	G983	S849	F787	F787
	G1178	S1118		A984	V921	LEU	LEU
	G1179	P1119	R1057	I985	L922	SER	SER
	W1180	L1120	L1058	K986	K923	GLU	GLU
	V1181	H1121	L1059	I987	Q924	ASP	ASP
	T1182	E1122	S1060	I988	E925	PRO	PRO
	L1183	L1123	W1061	E989	I926	GLU	GLU
	V1184	K1124	S1062	L990	D927	D796	D796
	C1185	G1125	F1063	P991	V928	V797	V797
	F1186	H1126	D1064	R992	S860	E798	E798
	S1187	N1127	G1065	R993	Q861	V799	V799
	P1188	G1128	T1066	R994	Y862	I800	I800
	D1189	C1129	V1067	V995	C863	V801	V801
	S1190	V1130	K1068	S998	V864	K802	K802
	K1191	R1131	V1069		E934	C803	C803
	T1192	C1132	W1070	G1001	M867	C804	C804
	L1193	S1133	M1071	H1002	M868	S865	S865
	V1194	F1135	V1072	K1003	A939	W806	W806
		I1136	I1073		D870	D809	D809
	K1201	S1137	T1074	V1006	S871		
	W1202	D1138	G1075	R1007	I943		
	W1203	G1139	A1076	H1008	R944		
	N1204	I1140	I1077	I1009	G945		
	V1205	E1078	R1079	Q1010			
	A1206	L1141					

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 48.85 – 3.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.55) 99.6 (48.85-3.55)	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 0.229 , 0.284	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)	0.32 , 78.6	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	0.91	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	0.45	0/9206	0.72	5/12465 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	761	CYS	CA-CB-SG	-6.36	102.55	114.00
1	A	922	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	460	MET	N-CA-C	-5.66	95.71	111.00
1	A	796	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	705	CYS	CA-CB-SG	5.06	123.12	114.00

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	902	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	902	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 50.

The worst 5 of 902 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:N	1:A:288:ARG:HE	1.58	1.00
1:A:785:ARG:HH11	1:A:785:ARG:HG3	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 7

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%)	911 (91%)	94 (9%)	8	37

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	752	SER
1	A	866	LEU
1	A	1137	LEU
1	A	784	LYS
1	A	826	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	ASN
1	A	868	ASN
1	A	1212	GLN
1	A	782	ASN
1	A	836	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	GBL	A	1252	-	6,6,6	0.69	0	7,7,7	0.77	0
3	GBL	A	1251	-	6,6,6	0.98	0	7,7,7	0.78	0
2	ADP	A	1250	-	24,29,29	1.44	3 (12%)	29,45,45	1.80	4 (13%)

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
3	GBL	A	1252	-	-	-	0/1/1/1
3	GBL	A	1251	-	-	-	0/1/1/1
2	ADP	A	1250	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ADP	O4'-C1'	4.19	1.46	1.41
2	A	1250	ADP	PB-O3B	2.37	1.64	1.54
2	A	1250	ADP	C6-N6	2.04	1.41	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ADP	PA-O3A-PB	-5.73	113.15	132.83
2	A	1250	ADP	N3-C2-N1	-4.48	121.67	128.68
2	A	1250	ADP	C3'-C2'-C1'	3.31	105.95	100.98
2	A	1250	ADP	C4-C5-N7	-2.35	106.95	109.40

There are no chirality outliers.

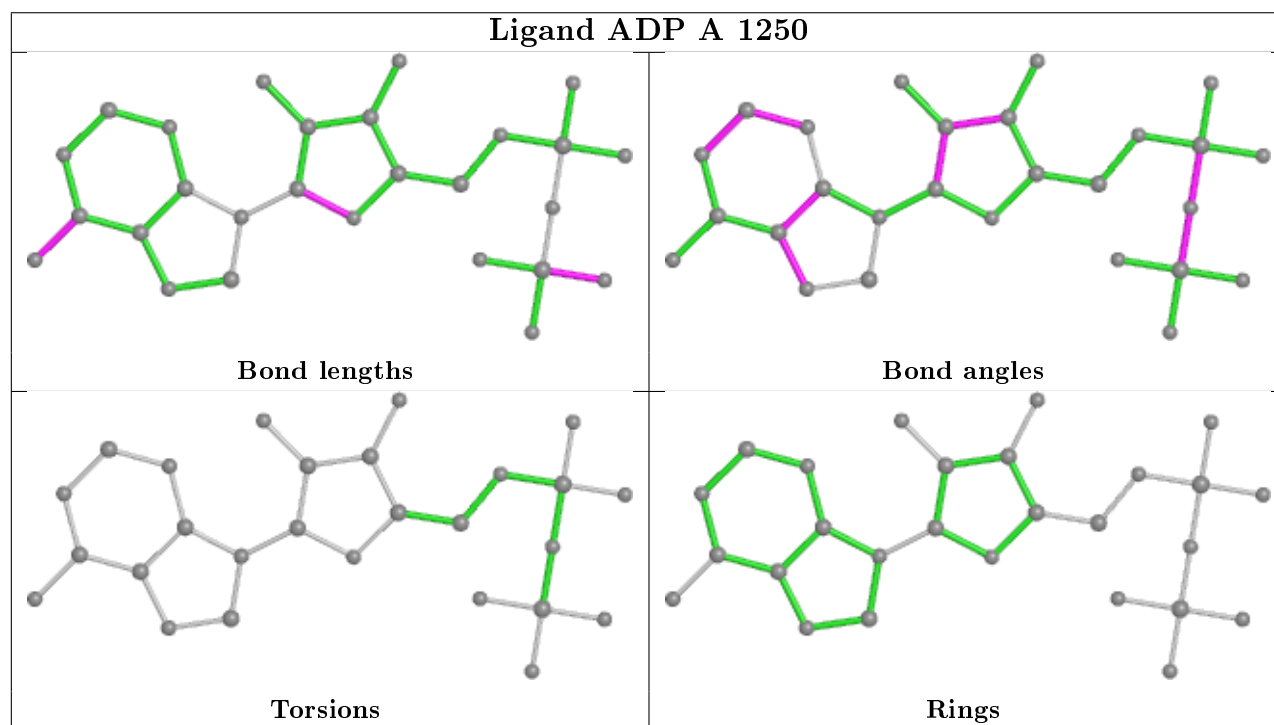
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1251	GBL	1	0
2	A	1250	ADP	3	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 [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	A	1133/1256 (90%)	-0.14	13 (1%) 80 67	74, 106, 140, 175	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	5.2
1	A	102	THR	4.7
1	A	1124	LYS	4.3
1	A	1177	HIS	3.9
1	A	104	GLY	3.4

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

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

6.3 Carbohydrates [i](#)

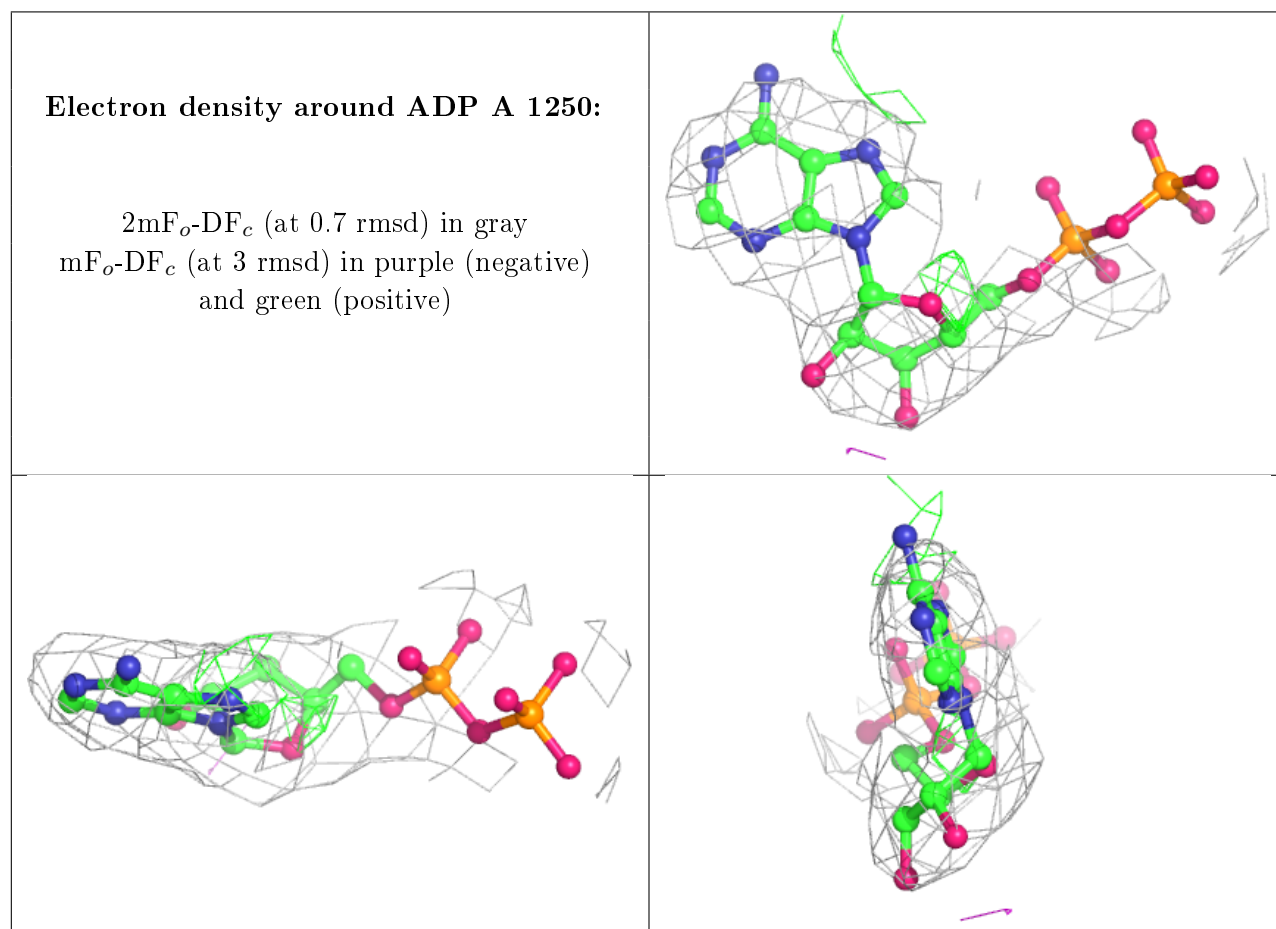
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	GBL	A	1251	6/6	0.92	0.26	91,92,92,93	0
2	ADP	A	1250	27/27	0.94	0.21	81,86,90,90	0
3	GBL	A	1252	6/6	0.96	0.24	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.