wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 05:06 AM EDT

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 (i) 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 (i)) were used in the production of this report:

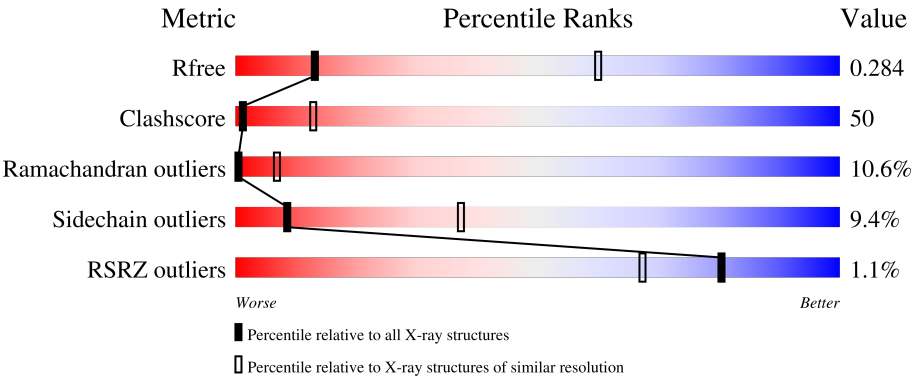
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.55 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 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 <=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	% 29% 48% 12% • 10%

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.

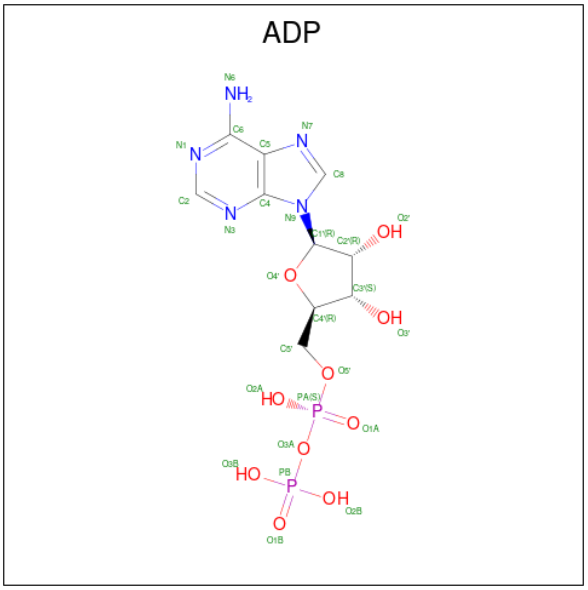
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

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

There are 8 discrepancies between the modelled and reference sequences:

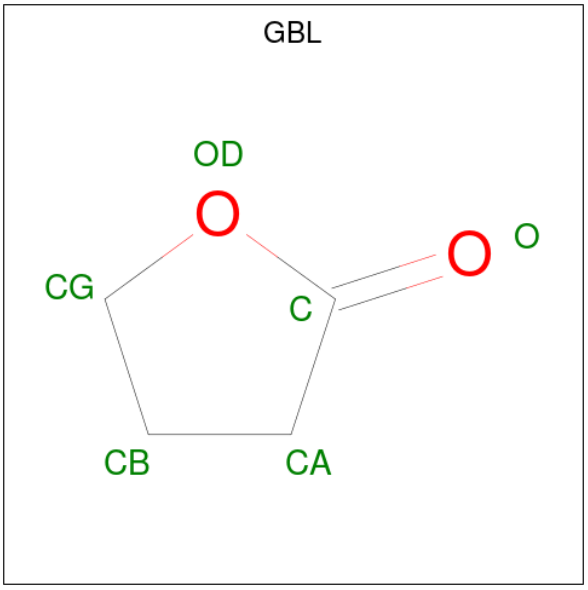
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A2RRK8
A	-5	ALA	-	expression tag	UNP A2RRK8
A	-4	MET	-	expression tag	UNP A2RRK8
A	-3	ASP	-	expression tag	UNP A2RRK8
A	-2	PRO	-	expression tag	UNP A2RRK8
A	-1	GLU	-	expression tag	UNP A2RRK8
A	0	PHE	-	expression tag	UNP A2RRK8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

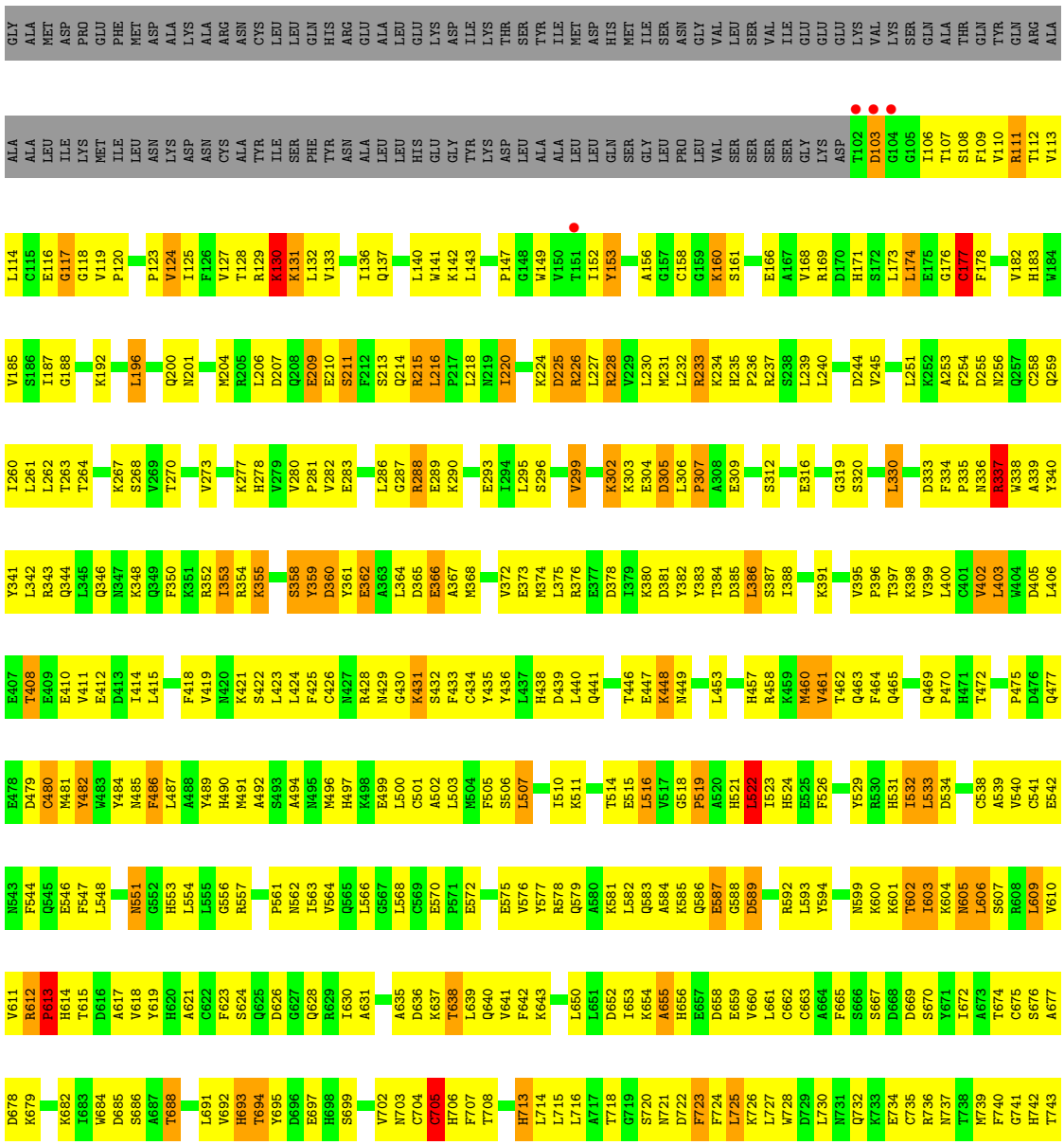
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		

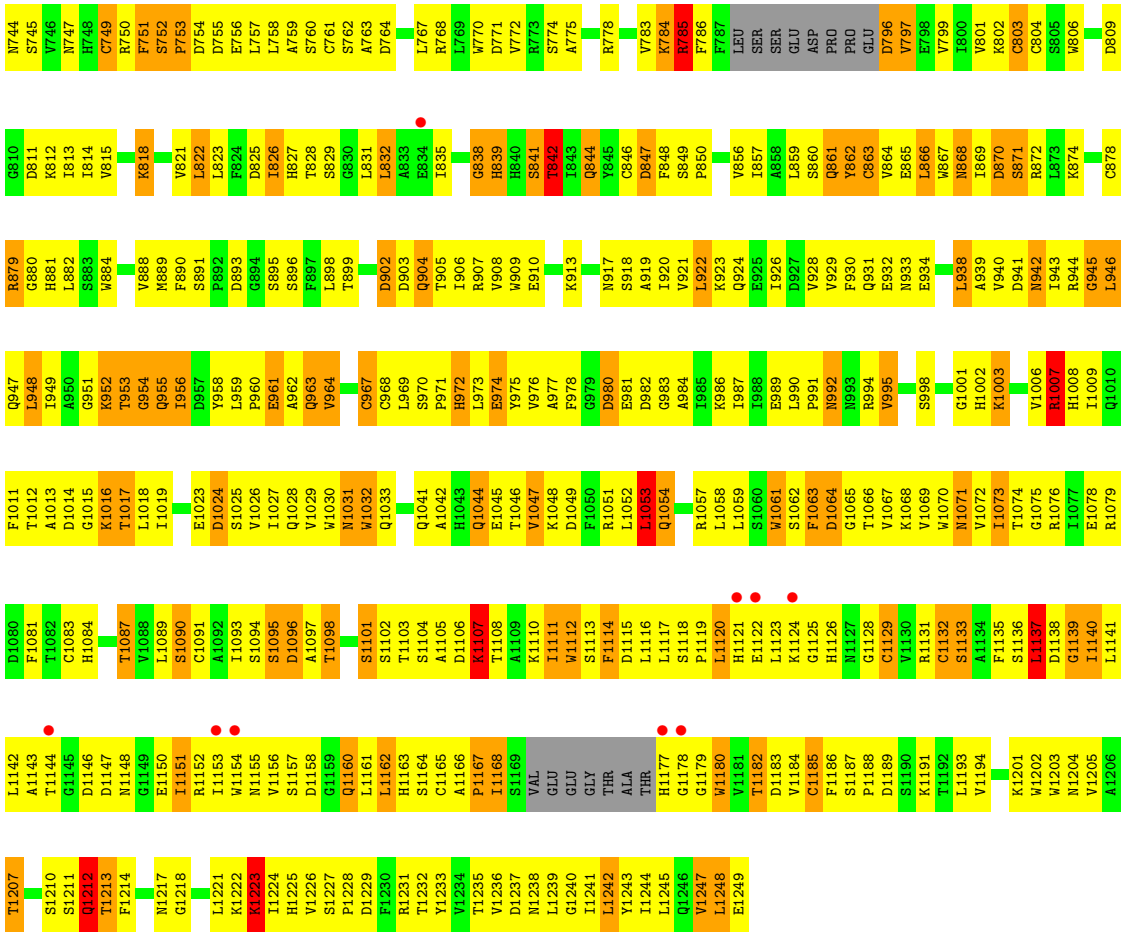
3 Residue-property plots (i)

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

Chain A:




N744 S745 V746 N747 H748 C749 R750 F751 S752 P753 D754 D755 E756 L757 L758 A759 S760 C761 S762 A763 D764 L767 R768 L769 W770 D771 V772 R773 S774 A775 R778 V783 K784 R785 F786 F787 LEU SER SER GLU ASP PRO PRO GLU D796 V797 E798 V799 I800 V801 K802 C803 C804 S805 W806 D809
G810 D811 K812 I813 I814 V815 K818 V821 L822 L823 P824 D825 I826 H827 T828 S829 G830 L831 L832 A833 E834 I835 G838 H839 H840 S841 T842 I843 Q844 Y845 C846 D847 F848 S849 P850 V856 I857 A858 L859 S860 Q861 Y862 C863 V864 E865 L866 W867 N868 I869 D870 S871 R872 L873 K874 C878
R879 G880 H881 L882 S883 W884 V888 M889 F890 S891 P892 D893 G894 S895 S896 F897 L898 T899 D902 D903 Q904 T905 I906 R907 V908 W909 E910 K913 N917 S918 A919 I920 V921 L922 K923 Q924 E925 I926 D927 V928 V929 F930 Q931 E932 N933 E934 L938 A939 V940 D941 N942 I943 R944 G945 L946
Q947 L948 I949 A950 G951 K952 T953 G954 Q955 I956 D957 Y958 L959 P960 E961 A962 Q963 V964 C967 C968 L969 S970 P971 H972 L973 E974 Y975 V976 A977 F978 G979 D980 E981 D982 G983 A984 I985 K986 I987 I988 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 N1031 W1032 Q1033 Q1041 A1042 H1043 Q1044 E1045 T1046 V1047 K1048 D1049 F1050 R1051 L1052 L1053 Q1054 R1057 L1058 L1059 S1060 W1061 S1062 F1063 D1064 G1065 T1066 V1067 K1068 V1069 W1070 N1071 V1072 I1073 T1074 G1075 R1076 I1077 E1078 R1079
D1080 F1081 T1082 C1083 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 D1115 L1116 L1117 S1118 P1119 L1120 H1121 E1122 L1123 K1124 G1125 H1126 N1127 G1128 C1129 V1130 R1131 C1132 S1133 A1134 F1135 S1136 L1137 D1138 G1139 I1140 L1141
L1142 A1143 T1144 G1145 D1146 D1147 N1148 G1149 E1150 I1151 R1152 I1153 W1154 N1155 V1156 S1157 D1158 G1159 Q1160 L1161 L1162 H1163 S1164 C1165 A1166 P1167 I1168 S1169 VAL GLU GLU GLY THR ALA THR H1177 G1178 G1179 W1180 V1181 T1182 D1183 V1184 C1185 F1186 S1187 P1188 D1189 S1190 K1191 T1192 L1193 V1194 K1201 W1202 W1203 N1204 V1205 A1206
T1207 S1210 S1211 Q1212 T1213 F1214 N1217 G1218 L1221 K1222 K1223 I1224 H1225 V1226 S1227 P1228 D1229 F1230 R1231 T1232 Y1233 V1234 T1235 V1236 D1237 N1238 L1239 G1240 I1241 L1242 Y1243 I1244 L1245 Q1246 V1247 L1248 E1249

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ADP, GBL

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(^{o})	Ideal(^{o})
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

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: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 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	902	ASP
1	A	1007	ARG
1	A	922	LEU
1	A	963	GLN
1	A	1041	GLN

Sometimes 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	1002	HIS
1	A	1177	HIS
1	A	1008	HIS
1	A	1071	ASN
1	A	1217	ASN

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 monosaccharides 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	1251	-	6,6,6	0.98	0	7,7,7	0.78	0
3	GBL	A	1252	-	6,6,6	0.69	0	7,7,7	0.77	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	1251	-	-	-	0/1/1/1
3	GBL	A	1252	-	-	-	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(^{o})	Ideal(^{o})
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.

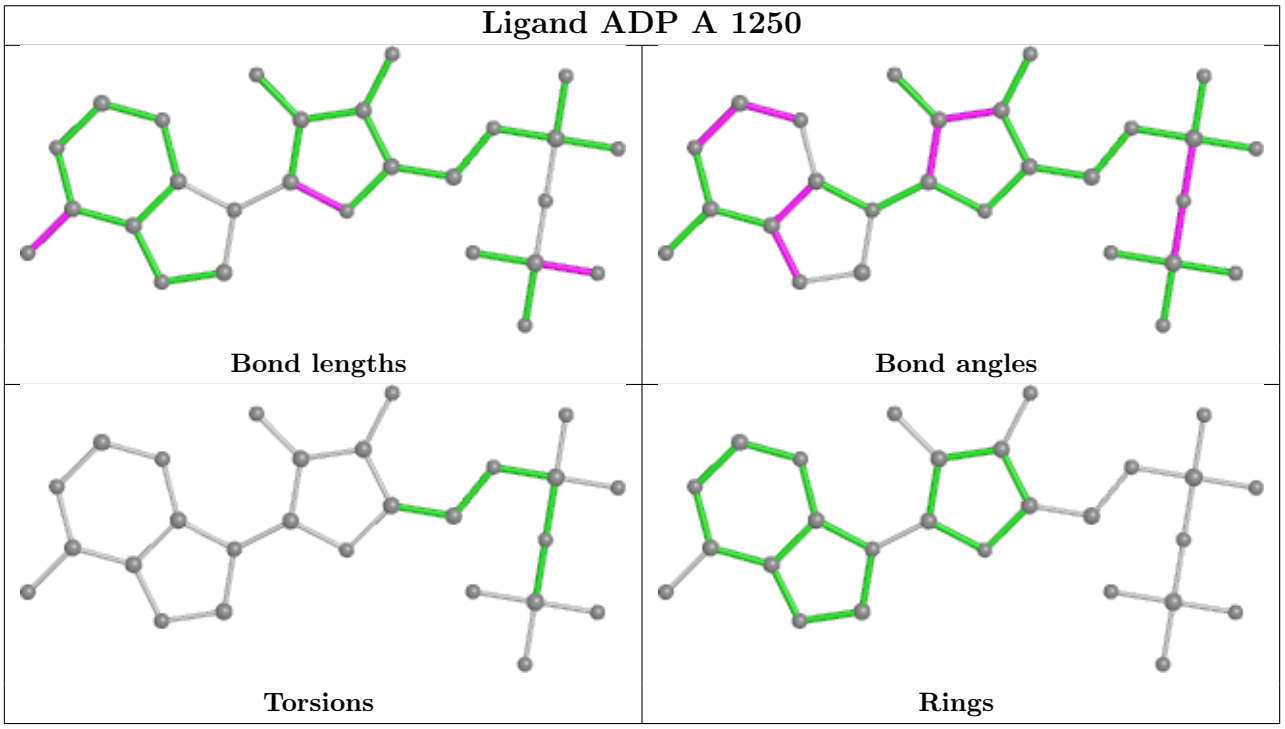
There are no torsion outliers.

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 then 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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

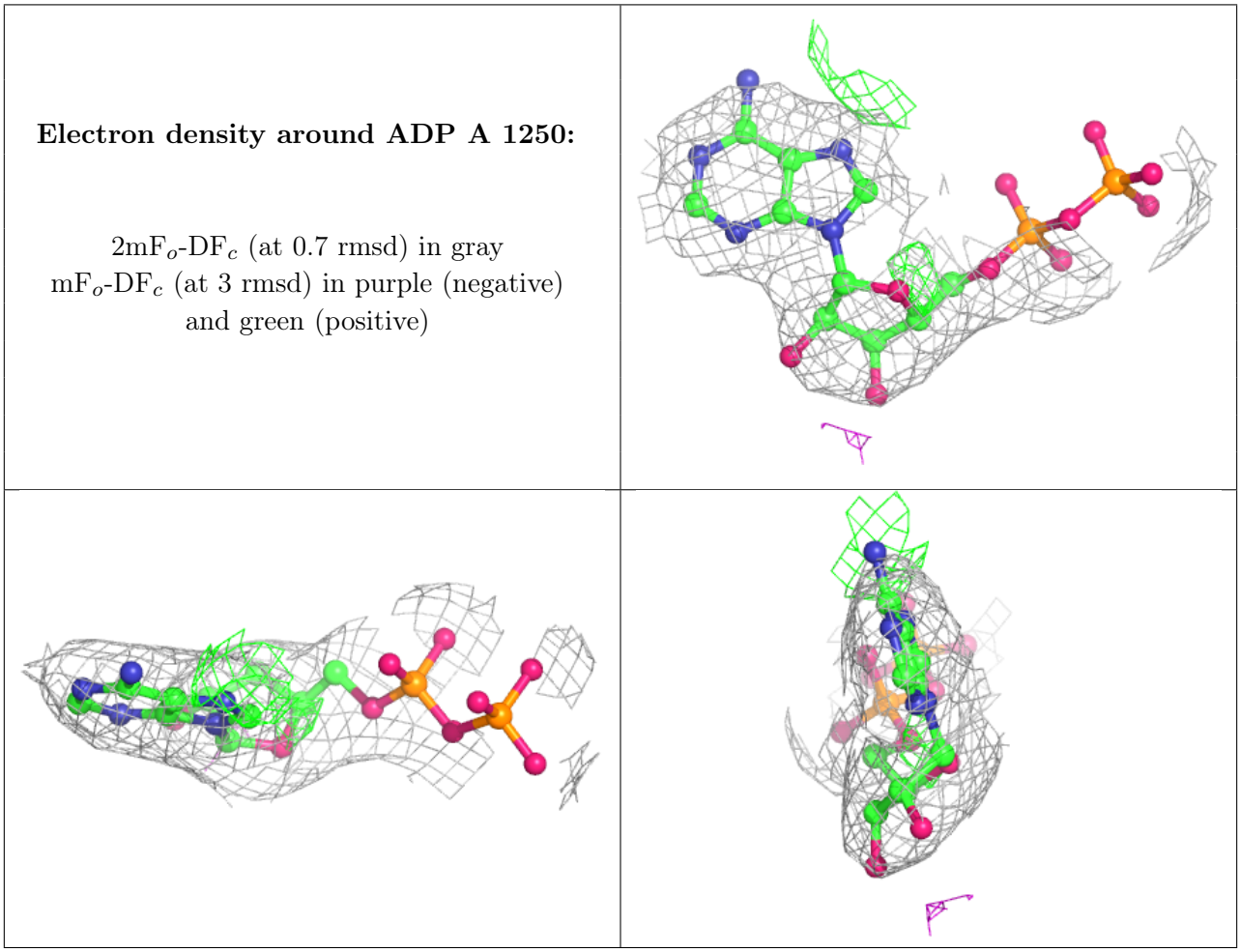
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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.

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.