



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:01 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

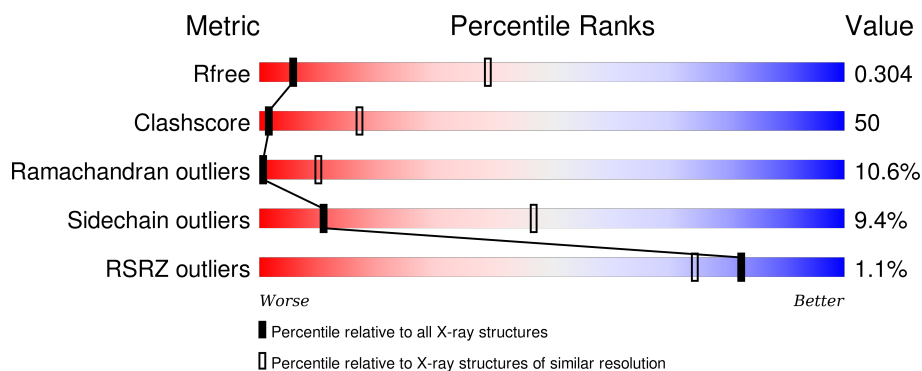
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

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. 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.

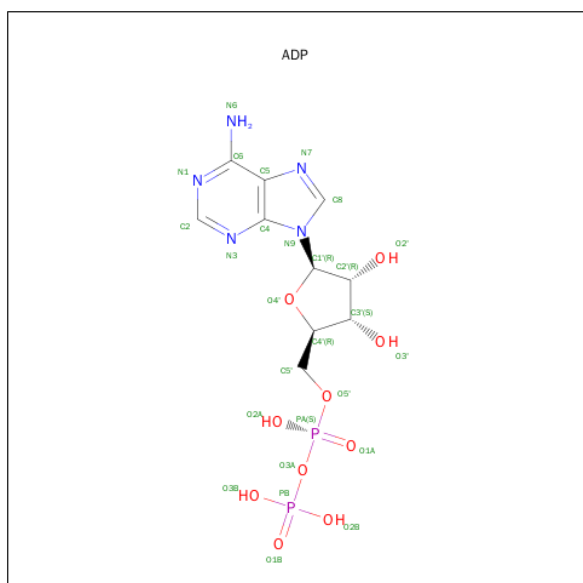
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

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:

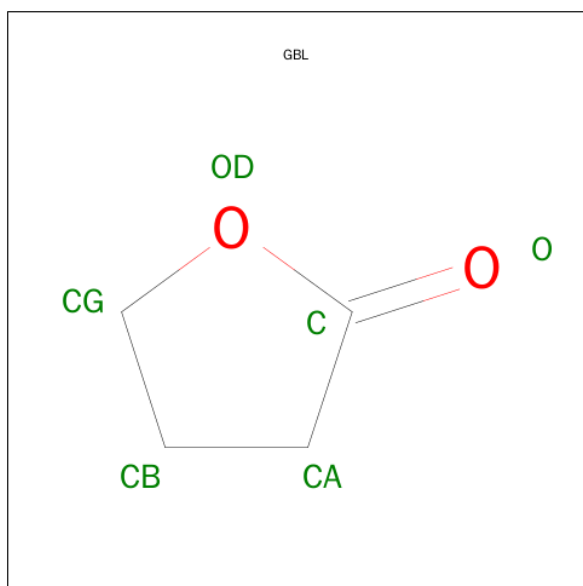
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	EXPRESSION TAG	UNP A2RRK8
A	-5	ALA	-	EXPRESSION TAG	UNP A2RRK8
A	-4	MET	-	EXPRESSION TAG	UNP A2RRK8
A	-3	ASP	-	EXPRESSION TAG	UNP A2RRK8
A	-2	PRO	-	EXPRESSION TAG	UNP A2RRK8
A	-1	GLU	-	EXPRESSION TAG	UNP A2RRK8
A	0	PHE	-	EXPRESSION TAG	UNP A2RRK8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

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (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: C₄H₆O₂).



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		

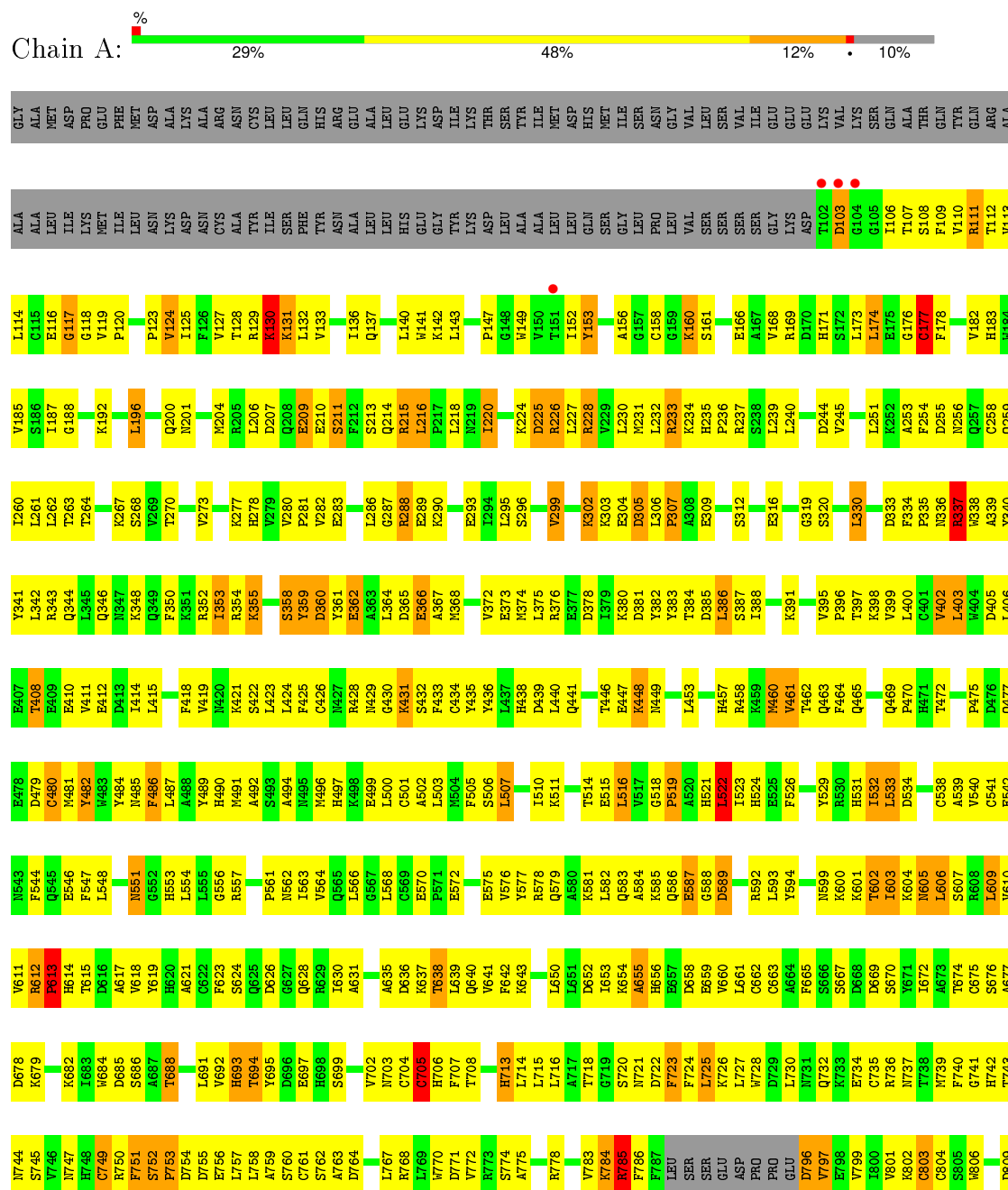
- Molecule 4 is water.

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 errors 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 ($\text{RSRZ} > 2$). 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



Tl207	L1142	B1080	F1011	Q947	B879	G810
S1210	A1143	F1081	Tl012	L948	G880	D811
S1211	Tl144	Tl082	A1013	L949	B881	K812
Q1212	G1145	C1083	D1014	A950	L882	I813
Tl213	D1146	H1084	G1015	S883	I814	V815
F1214	D1147		K1016	K952	W884	
	N1148	Tl087	Tl017	T853		K818
	G1149	V1088	L1018	G954	V888	
N1217	E1150	L1089	L1019	Q955	M889	
G1218	Tl151	S1090		F890	F891	V821
	L1152	C1091	E1023	D957	S891	L822
L1221	Tl153	A1092	D1024	Y958	F892	L823
K1222	H1154	I1093	S1025	L859	D893	F824
K1223	N1155	S1094	V1026	P860	G894	D825
H1224	V1156	S1095	Tl027	E961	S895	I826
H1225	D1096	D1096	Q1028	A962	S896	H827
V1226	S1157	A1097	V1029	Q963	F897	T828
S1227	G1159	Tl098	W1030	V964	L898	S829
P1228	Q1160		N1031		T899	G830
D1229	L1161	S1101	W1032	C967		L831
F1230	L1162	S1102	Q1033	C968	D902	L832
R1231	H1163	Tl103		L969	D903	A833
Tl232	S1164	S1104	Q1041	S970	Q904	E834
V1233	C1165	A1105	A1042	P971	T905	I835
V1234	A1166	D1106	H1043	H972	T906	
Tl235	P1167	K1107	Q1044	L973	R907	G838
V1236	Tl168	Tl108	E1045	E974	V908	H839
D1237	S1169	A1109	Tl046	Y975	W909	H840
N1238	VAL	K1110	V1047	V976	E910	S841
L1239	GLU	I1111	K1048	A977		T842
G1240	GLU	W1112	D1049	F978		I843
Tl241	GLY	S1113	F1050	G979		Q844
L1242	THR	F1114	A1051	D980	N917	T845
Y1243	ALA	D1115	L1052	E981	S918	C946
L1244	THR	L1116	L1053	D982	A919	D847
L1245		L1117	Q1054	G983	I920	F848
Q1246	H1177	S1118		A984	V921	S949
V1247	G1178	P1119	R1057	T985	I922	P850
L1248	G1179	L1120	L1058	K986	K923	
E1249	W1180	H1121	L1059	L987	Q924	V856
	Tl181	E1122	S1060	F988	E925	I857
	D1183	L1123	W1061	E989	I926	A858
	V1184	K1124	S1062	L990	D927	L859
	G1185	G1125	F1063	P991	V928	S860
	F1186	H1126	D1064	N992	V929	Q861
	S1187	M1127	G1065	N993	F930	Y862
	P1188	G1128	Tl066	R994	Q931	C863
	D1189	C1129	V1067	V995	E932	V864
	S1190	V1130	K1068		N933	E865
	K1191	R1131	V1069	S998	E934	L866
	Tl192	C1132	W1070		W867	
	L1193	S1133	N1071	G1001	L988	N868
	V1194	A1134	V1072	H1002	A939	I869
		F1135	Tl073	K1003	V940	D870
	K1201	S1136	Tl074	V1006	D941	S871
	W1202	L1137	G1075	R1007	N942	R872
	W1203	D1138	A1076	I1007	I943	L873
	N1204	G1139	Tl077	H1008	R944	K874
	W1205	Tl140	E1078	Tl009	G945	
	A1206	L1141	R1079	Q1010	L946	C878

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 0.230 , 0.304	Depositor DCC
R_{free} test set	987 reflections (4.00%)	DCC
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 , 78.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 201873 reflections	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, 0.375 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: 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	10

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%)	11	47

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 ⓘ

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 ⓘ

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	-	22,29,29	1.57	4 (18%)	27,45,45	2.52	5 (18%)
3	GBL	A	1251	-	6,6,6	1.03	0	7,7,7	0.91	1 (14%)
3	GBL	A	1252	-	6,6,6	0.72	0	7,7,7	0.90	1 (14%)

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	-	-	0/12/32/32	0/3/3/3
3	GBL	A	1251	-	-	0/0/7/7	0/1/1/1
3	GBL	A	1252	-	-	0/0/7/7	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ADP	PA-O2A	2.07	1.63	1.54
2	A	1250	ADP	C6-N6	2.11	1.41	1.34
2	A	1250	ADP	PB-O3B	2.58	1.64	1.54
2	A	1250	ADP	O4'-C1'	4.53	1.46	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ADP	N3-C2-N1	-9.43	121.67	128.89
2	A	1250	ADP	PA-O3A-PB	-5.82	113.15	132.67
2	A	1250	ADP	C2'-C1'-N9	-4.17	107.93	114.29
2	A	1250	ADP	C4-C5-N7	-2.75	106.95	109.48
3	A	1251	GBL	OD-C-O	2.12	125.00	120.25

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

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%)	-0.11	13 (1%) 82 74	74, 106, 140, 175	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASP	5.3
1	A	102	THR	4.7
1	A	1124	LYS	4.2
1	A	1177	HIS	3.8
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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	GBL	A	1251	6/6	0.92	0.26	0.57	91,92,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GBL	A	1252	6/6	0.96	0.24	0.55	100,101,102,103	0
2	ADP	A	1250	27/27	0.94	0.21	-0.15	81,86,90,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.