



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2016 – 09:01 PM EDT

PDB ID : 5FTC
Title : Crystal structure of Pif1 helicase from Bacteroides in complex with ADP
Authors : Chen, W.-F.; Dai, Y.-X.; Duan, X.-L.; Liu, N.-N.; Shi, W.; Li, M.; Dou, S.-X.;
Li, N.; Dong, Y.-H.; Rety, S.; Xi, X.-G.
Deposited on : 2016-01-12
Resolution : 2.27 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
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) : rb-20027107

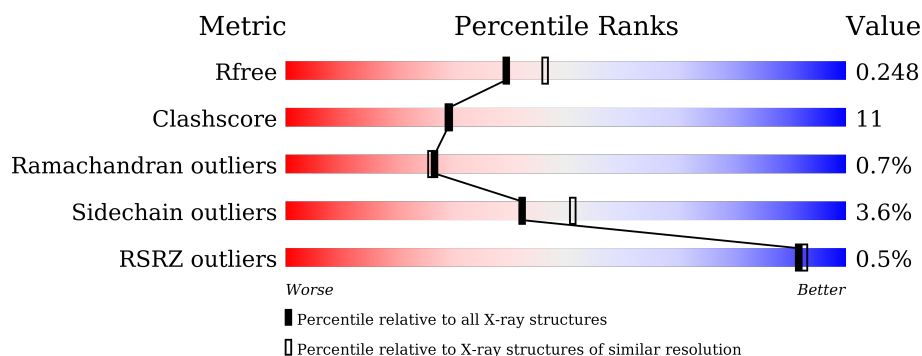
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	433	<div> <div style="width: 81%; background-color: green;"></div> <div style="width: 17%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: red;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <div>81% 17% .</div>

2 Entry composition [i](#)

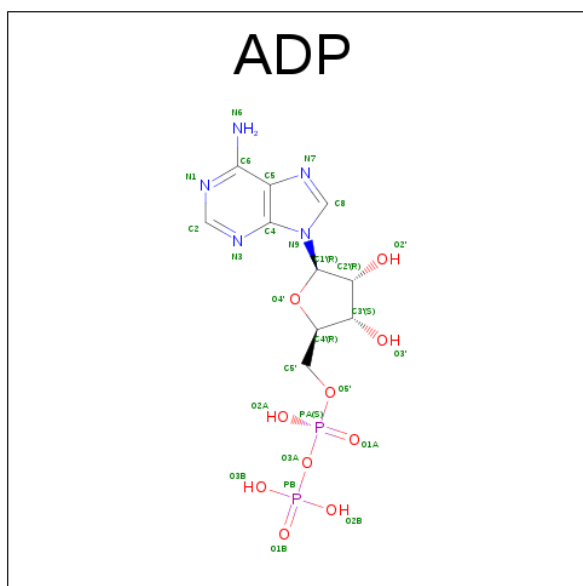
There are 4 unique types of molecules in this entry. The entry contains 3597 atoms, of which 12 are hydrogens and 0 are deuteriums.

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 TPR DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	1
			3481	2236	573	655	17			

- 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	H	N	O	P	0	0
			39	10	12	5	10	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		

- Molecule 1: TPR DOMAIN PROTEIN

S376	H377	T378	F379	C380	C391	L394	E395	A401	K405	Y421	L422	ASP	K185	P192	E193	F194	M195	L196	V197	N198	R202	T207	E210	L211	R220	K221	D227	T233	C234	T235	E236	K237	K262	D272	R282	L291	V302	A304	L305	T311	T333	L334	K335	D336	Q349	F350	T359	I360	I371	P375	T180	K185	P192	E193	F194	M195	L196	V197	N198	R202	T207	E210	L211	R220	K221	D227	T233	C234	T235	E236	K237	K262	D272	R282	L291	V125	S128	I138	M139	F144	Q145	L146	P147	K148	V149	T150	K151	F152	Q153	E154	R155	E156	I157	T160	K165	P166	E167	F168	M169	L170	V171	N172	R173	K174	D175	T176	E177	L178	R179	K180	D181	T182	E183	L184	R185	K186	K187	M188	V189	N190	R191	K192	D193	T194	E195	L196	R197	K198	D199	T200	E201	L202	R203	K204	D205	T206	E207	L208	R209	K210	D211	T212	E213	L214	R215	K216	D217	T218	E219	L220	R221	K222	D223	T224	E225	L226	R227	K228	D229	T230	E231	L232	R233	K234	D235	T236	E237	L238	R239	K240	D241	T242	E243	L244	R245	K246	D247	T248	E249	L250	R251	K252	D253	T254	E255	L256	R257	K258	D259	T260	E261	L262	R263	K264	D265	T266	E267	L268	R269	K270	D271	T272	E273	L274	R275	K276	D277	T278	E279	L280	R281	K282	D283	T284	E285	L286	R287	K288	D289	T290	E291	L292	R293	K294	D295	T296	E297	L298	R299	K300	D301	T302	E303	L304	R305	K306	D307	T308	E309	L310	R311	K312	D313	T314	E315	L316	R317	K318	D319	T320	E321	L322	R323	K324	D325	T326	E327	L328	R329	K330	D331	T332	E333	L334	R335	K336	D337	T338	E339	L340	R341	K342	D343	T344	E345	L346	R347	K348	D349	T350	E351	L352	R353	K354	D355	T356	E357	L358	R359	K360	D361	T362	E363	L364	R365	K366	D367	T368	E369	L370	R371	K372	D373	T374	E375	L376	R377	K378	D379	T380	E381	L382	R383	K384	D385	T386	E387	L388	R389	K390	D391	T392	E393	L394	R395	K396	D397	T398	E399	L400	R401	K402	D403	T404	E405	L406	R407	K408	D409	T410	E411	L412	R413	K414	D415	T416	E417	L418	R419	K420	D421	T422	E423	L424	R425	K426	D427	T428	E429	L430	R431	K432	D433	T434	E435	L436	R437	K438	D439	T440	E441	L442	R443	K444	D445	T446	E447	L448	R449	K450	D451	T452	E453	L454	R455	K456	D457	T458	E459	L460	R461	K462	D463	T464	E465	L466	R467	K468	D469	T470	E471	L472	R473	K474	D475	T476	E477	L478	R479	K480	D481	T482	E483	L484	R485	K486	D487	T488	E489	L490	R491	K492	D493	T494	E495	L496	R497	K498	D499	T500	E501	L502	R503	K504	D505	T506	E507	L508	R509	K510	D511	T512	E513	L514	R515	K516	D517	T518	E519	L520	R521	K522	D523	T524	E525	L526	R527	K528	D529	T530	E531	L532	R533	K534	D535	T536	E537	L538	R539	K540	D541	T542	E543	L544	R545	K546	D547	T548	E549	L550	R551	K552	D553	T554	E555	L556	R557	K558	D559	T560	E561	L562	R563	K564	D565	T566	E567	L568	R569	K570	D571	T572	E573	L574	R575	K576	D577	T578	E579	L580	R
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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	67.17Å 74.03Å 109.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.21 – 2.27 57.21 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (57.21-2.27) 100.0 (57.21-2.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.27Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.195 , 0.249 0.191 , 0.248	Depositor DCC
R_{free} test set	1343 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 25853 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3597	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.42	0/3550	0.54	0/4796

There are no bond length outliers.

There are no bond angle outliers.

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	3481	0	3496	80	0
2	A	27	12	12	1	0
3	A	2	0	0	0	0
4	A	75	0	0	7	0
All	All	3585	12	3508	80	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 11.

All (80) 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:146:LEU:HD12	1:A:147:PRO:HD2	1.35	1.06
1:A:6:LEU:HA	1:A:10:MET:HE1	1.52	0.90
1:A:6:LEU:HA	1:A:10:MET:CE	2.02	0.89
1:A:146:LEU:CD1	1:A:147:PRO:HD2	2.04	0.87
1:A:101:LEU:HD11	1:A:138:ILE:HG12	1.59	0.85
1:A:85:GLU:HB3	1:A:87:LYS:HE2	1.62	0.81
1:A:272:ASP:OD2	4:A:2052:HOH:O	2.00	0.78
1:A:311:THR:OG1	4:A:2058:HOH:O	2.01	0.77
1:A:194:PHE:HD1	1:A:394:LEU:HD13	1.50	0.75
1:A:235:THR:HG22	1:A:360:ILE:CD1	2.16	0.75
1:A:262:ASP:O	4:A:2048:HOH:O	2.05	0.74
1:A:235:THR:HG22	1:A:360:ILE:HD12	1.73	0.71
1:A:6:LEU:HD12	1:A:10:MET:CE	2.22	0.70
1:A:302:VAL:HG11	1:A:305:LEU:HD21	1.73	0.69
1:A:6:LEU:HD12	1:A:10:MET:HE3	1.74	0.67
1:A:7:THR:H	1:A:10:MET:CE	2.10	0.65
1:A:5:ILE:O	1:A:10:MET:HE1	1.96	0.65
1:A:7:THR:H	1:A:10:MET:HE2	1.62	0.65
1:A:121:LYS:O	1:A:125:VAL:HG12	1.97	0.64
1:A:85:GLU:HG2	1:A:87:LYS:NZ	2.14	0.62
1:A:50:ILE:HB	1:A:99:MET:CE	2.29	0.62
1:A:379:PHE:HD2	1:A:380:CYS:H	1.48	0.62
1:A:193:GLU:H	1:A:193:GLU:CD	2.03	0.62
1:A:150:THR:HA	1:A:154:GLU:OE2	2.00	0.61
1:A:50:ILE:HD12	1:A:99:MET:HE2	1.82	0.61
1:A:38:LEU:HD11	1:A:103:ILE:HG21	1.85	0.59
1:A:291:LEU:HD13	1:A:291:LEU:O	2.03	0.58
1:A:192:PRO:O	1:A:195:ILE:HG22	2.02	0.57
1:A:237:LYS:HD2	1:A:359:THR:HG21	1.86	0.57
1:A:211:LEU:HD21	1:A:405:LYS:HB2	1.86	0.57
1:A:84:LEU:HD21	1:A:120:ARG:CZ	2.36	0.56
1:A:180:ILE:HD12	1:A:180:ILE:N	2.21	0.56
1:A:375:VAL:HG21	1:A:401:ALA:HB3	1.87	0.56
1:A:375:VAL:HG23	1:A:377:HIS:CD2	2.42	0.55
1:A:50:ILE:HB	1:A:99:MET:HE1	1.88	0.54
1:A:375:VAL:HG23	1:A:377:HIS:NE2	2.22	0.53
1:A:233:ILE:HD12	1:A:371:ILE:HB	1.90	0.53
1:A:194:PHE:CD1	1:A:394:LEU:HD13	2.38	0.53
1:A:421:TYR:OH	4:A:2038:HOH:O	2.19	0.53
1:A:235:THR:HG22	1:A:360:ILE:HD13	1.93	0.51
1:A:193:GLU:O	1:A:197:VAL:HG23	2.11	0.51
1:A:199:ASN:HA	1:A:202:ARG:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLN:O	1:A:157:ILE:HD13	2.12	0.50
1:A:50:ILE:HB	1:A:99:MET:HE2	1.93	0.50
1:A:144:PHE:CE2	1:A:202:ARG:HD3	2.47	0.50
1:A:151:LYS:HB2	1:A:154:GLU:HG2	1.94	0.49
1:A:235:THR:CG2	1:A:360:ILE:HD12	2.40	0.49
1:A:29:LYS:HE3	1:A:202:ARG:NH2	2.28	0.49
1:A:379:PHE:CD2	1:A:380:CYS:N	2.79	0.49
1:A:50:ILE:HD12	1:A:99:MET:CE	2.43	0.49
1:A:221:LYS:HB2	4:A:2043:HOH:O	2.13	0.49
1:A:262:ASP:O	4:A:2050:HOH:O	2.20	0.47
1:A:349:GLN:HG3	1:A:350:PHE:N	2.29	0.47
1:A:10:MET:HE2	1:A:10:MET:HB2	1.65	0.47
1:A:395:GLU:N	1:A:395:GLU:OE1	2.41	0.47
1:A:335:LYS:O	1:A:336:ASP:HB2	2.14	0.47
1:A:304:ALA:HB3	1:A:311:THR:HB	1.97	0.46
1:A:157:ILE:N	1:A:157:ILE:HD12	2.31	0.46
1:A:50:ILE:CG1	1:A:99:MET:HE2	2.45	0.46
1:A:207:THR:OG1	1:A:210:GLU:HG3	2.15	0.46
1:A:146:LEU:CG	1:A:147:PRO:HD2	2.45	0.45
1:A:6:LEU:CA	1:A:10:MET:HE1	2.34	0.45
1:A:371:ILE:HD13	1:A:391:CYS:HB2	1.99	0.45
1:A:147:PRO:HB2	1:A:148:PRO:HD2	1.97	0.45
1:A:291:LEU:HD13	1:A:291:LEU:C	2.38	0.45
1:A:107:ILE:HG12	1:A:139:MET:HE1	1.99	0.45
1:A:50:ILE:CD1	1:A:99:MET:HE2	2.48	0.44
1:A:107:ILE:CD1	1:A:139:MET:HE2	2.47	0.44
1:A:153:GLN:HA	1:A:153:GLN:OE1	2.18	0.44
1:A:4:MET:HG3	2:A:1432:ADP:N6	2.32	0.43
1:A:84:LEU:N	1:A:84:LEU:HD22	2.32	0.43
1:A:101:LEU:HD11	1:A:138:ILE:CG1	2.40	0.43
1:A:146:LEU:HD12	1:A:147:PRO:CD	2.26	0.42
1:A:29:LYS:HE3	1:A:202:ARG:HH21	1.84	0.42
1:A:263:LYS:HA	4:A:2050:HOH:O	2.18	0.42
1:A:333:THR:HG22	1:A:334:LEU:H	1.85	0.42
1:A:6:LEU:HD12	1:A:10:MET:HE2	2.01	0.41
1:A:40:TYR:CE1	1:A:44:LYS:HG3	2.55	0.41
1:A:7:THR:N	1:A:10:MET:HE2	2.32	0.41
1:A:85:GLU:HG2	1:A:87:LYS:HZ3	1.82	0.40

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	430/433 (99%)	413 (96%)	14 (3%)	3 (1%)	26	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	THR
1	A	379	PHE
1	A	380	CYS

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	388/390 (100%)	374 (96%)	14 (4%)	42	51

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	A	115	LEU
1	A	125	VAL
1	A	128	SER
1	A	150	THR
1	A	156	GLU
1	A	185	LYS
1	A	193	GLU

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Mol	Chain	Res	Type
1	A	195	ILE
1	A	202	ARG
1	A	220	ARG
1	A	227	ASP
1	A	282	ARG
1	A	333	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	383	GLN

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	1432	3	24,29,29	1.04	1 (4%)	23,45,45	1.85	2 (8%)

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	1432	3	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1432	ADP	C5-C4	3.14	1.47	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1432	ADP	N3-C2-N1	-7.56	122.93	128.87
2	A	1432	ADP	N6-C6-N1	2.23	122.26	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1432	ADP	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	432/433 (99%)	-0.28	2 (0%) 91 92	38, 64, 98, 121	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	85	GLU	2.1
1	A	146	LEU	2.1

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
2	ADP	A	1432	27/27	0.97	0.12	0.61	48,67,91,100	0
3	CA	A	1433	1/1	0.99	0.09	-	65,65,65,65	0
3	CA	A	1434	1/1	0.96	0.18	-	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.