



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 06:54 PM GMT

PDB ID : 2QPA
Title : Crystal Structure of S.cerevisiae Vps4 in the presence of ADP
Authors : Xiao, J.; Xu, Z.
Deposited on : 2007-07-23
Resolution : 3.20 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

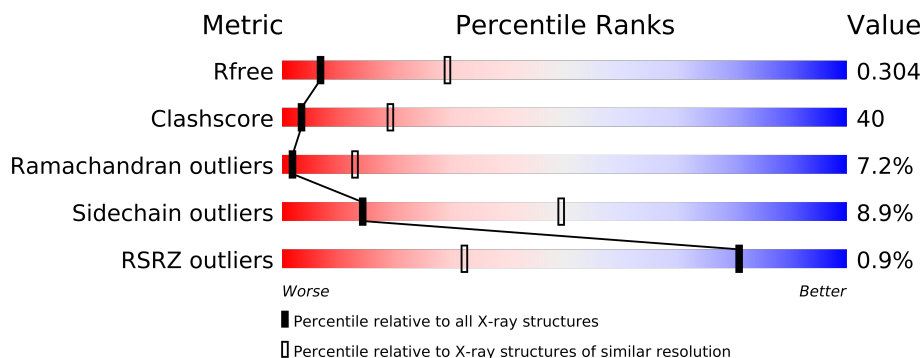
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	355	
1	B	355	
1	C	355	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	B	800	-	X
3	ADP	A	800	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6415 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Vacuolar protein sorting-associated protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2176	1388	364	418	6			
1	B	303	Total	C	N	O	S	0	0	0
			2120	1349	350	415	6			
1	C	296	Total	C	N	O	S	0	0	0
			2082	1327	342	407	6			

There are 9 discrepancies between the modelled and reference sequences:

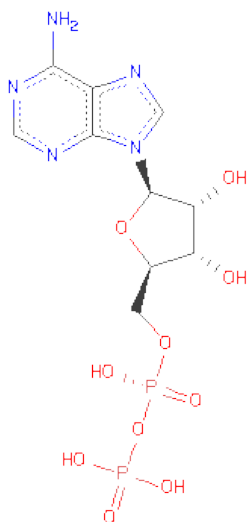
Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLN	GLU	ENGINEERED	UNP P52917
A	317	SER	CYS	ENGINEERED	UNP P52917
A	376	SER	CYS	ENGINEERED	UNP P52917
B	233	GLN	GLU	ENGINEERED	UNP P52917
B	317	SER	CYS	ENGINEERED	UNP P52917
B	376	SER	CYS	ENGINEERED	UNP P52917
C	233	GLN	GLU	ENGINEERED	UNP P52917
C	317	SER	CYS	ENGINEERED	UNP P52917
C	376	SER	CYS	ENGINEERED	UNP P52917

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	O	P		0	0
			5	4	1			
2	C	1	Total	O	P		0	0
			5	4	1			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



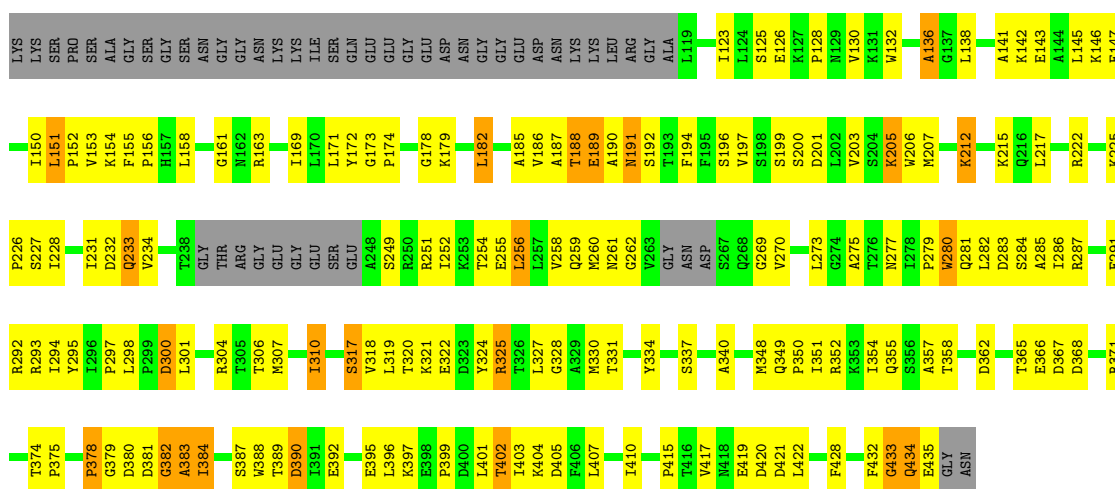
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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 ($RSRZ > 2$). 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.

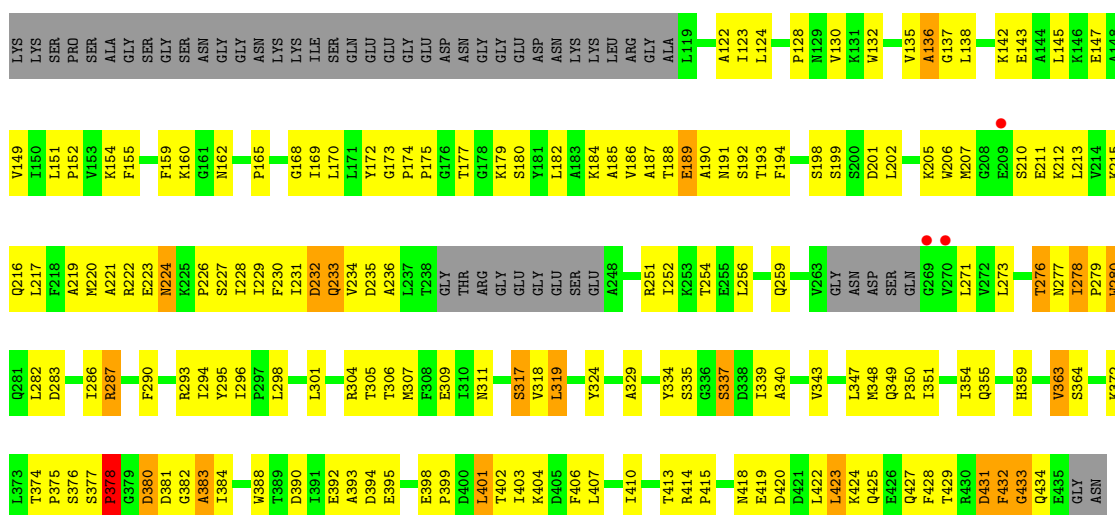
- Molecule 1: Vacuolar protein sorting-associated protein 4

Chain A:



- Molecule 1: Vacuolar protein sorting-associated protein 4

Chain B:



- Molecule 1: Vacuolar protein sorting-associated protein 4

Chain C: 

L347	K348	Q349	P350	I351	I354	Q355	T358	H359	F360	K361	T374	P375	S376	S377	P378	G382	A383	I384	E385	M386	A393	D394	E395	D400	L401	T402	I403	K404	L407	I410	T413	R414	P415	T416	V417	N418	E419	D420	D421	L422	L423	R430	D431	F432	GLY	GLN	GLU	GLY	ASN								
W280	Q281	L282	D283		R287		F290	E291	R292	R293	I294	Y295	I296	P297	L298	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
K216	L145	L217	F218		R222		P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
Q216	K145	L217	F218		R222		P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227	I228	I229	I230	I231	D232	Q233	D234	L301	R304	T305	T306	M307	F308	E309	I310	N311	V312		T315	P316	S317	V318	L319	T320	K321	F322	D323	Y324	R325	T326	L327	G328	A329	M330	T331		Y334	S335	G336	S337	D338	I339	A340	V341	Y342	V343	K344	D345	A346
	L145						P226	S227																																																	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.63Å 120.64Å 157.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 47.16 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (50.00-3.20) 95.0 (47.16-3.20)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.255 , 0.305 0.254 , 0.304	Depositor DCC
R_{free} test set	1107 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	106.7	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 109.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 24221 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6415	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0.47	0/2215	0.68	1/3027 (0.0%)
1	B	0.41	0/2159	0.64	1/2959 (0.0%)
1	C	0.36	0/2121	0.58	1/2907 (0.0%)
All	All	0.42	0/6495	0.63	3/8893 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	378	PRO	N-CA-CB	5.58	110.00	103.30
1	C	378	PRO	N-CA-CB	5.48	109.88	103.30
1	A	378	PRO	N-CA-CB	5.45	109.84	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2176	0	2009	157	0
1	B	2120	0	1891	151	0
1	C	2082	0	1867	186	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	27	0	12	4	0
All	All	6415	0	5779	484	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 40.

The worst 5 of 484 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:149:VAL:HG13	1:B:271:LEU:HD12	1.29	1.14
1:C:124:LEU:HB3	1:C:196:SER:HB3	1.34	1.05
1:C:146:LYS:HA	1:C:150:ILE:HD13	1.36	1.04
1:B:172:TYR:HB2	1:B:279:PRO:HG3	1.50	0.94
1:B:413:THR:HG22	1:B:414:ARG:H	1.29	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	299/355 (84%)	229 (77%)	47 (16%)	23 (8%)	1	11
1	B	297/355 (84%)	217 (73%)	60 (20%)	20 (7%)	2	16
1	C	290/355 (82%)	213 (73%)	56 (19%)	21 (7%)	2	13
All	All	886/1065 (83%)	659 (74%)	163 (18%)	64 (7%)	2	13

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ALA
1	A	189	GLU
1	A	191	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	VAL
1	A	205	LYS

5.3.2 Protein sidechains ⓘ

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	204/298 (68%)	190 (93%)	14 (7%)	22	65
1	B	192/298 (64%)	175 (91%)	17 (9%)	14	49
1	C	191/298 (64%)	170 (89%)	21 (11%)	9	36
All	All	587/894 (66%)	535 (91%)	52 (9%)	14	49

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	317	SER
1	B	423	LEU
1	C	400	ASP
1	B	319	LEU
1	B	390	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	233	GLN
1	B	311	ASN
1	C	216	GLN
1	A	355	GLN
1	B	355	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
3	ADP	A	800	-	29,29,29	1.11	2 (6%)	45,45,45	2.25	9 (20%)
2	PO4	B	800	-	4,4,4	0.82	0	6,6,6	0.31	0
2	PO4	C	800	-	4,4,4	0.82	0	6,6,6	0.31	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
3	ADP	A	800	-	-	0/16/32/32	0/1/3/3
2	PO4	B	800	-	-	0/0/0/0	0/0/0/0
2	PO4	C	800	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	ADP	C8-N7	-2.08	1.30	1.34
3	A	800	ADP	O4'-C1'	2.03	1.44	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	800	ADP	N3-C2-N1	-8.63	121.50	128.71
3	A	800	ADP	PA-O3A-PB	-8.11	107.91	131.68
3	A	800	ADP	N3-C4-N9	5.40	135.18	125.43
3	A	800	ADP	C5-C4-N3	-2.93	119.32	125.70
3	A	800	ADP	C4'-O4'-C1'	-2.42	107.11	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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, 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	305/355 (85%)	-0.00	0 100 100	66, 94, 139, 157	0
1	B	303/355 (85%)	0.06	3 (0%) 79 29	69, 119, 163, 184	0
1	C	296/355 (83%)	0.25	5 (1%) 67 19	97, 143, 185, 192	0
All	All	904/1065 (84%)	0.10	8 (0%) 81 32	66, 122, 174, 192	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	LEU	3.5
1	B	209	GLU	3.3
1	C	194	PHE	3.0
1	C	360	PHE	2.6
1	B	269	GLY	2.5

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 carbohydrates 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. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	B	800	5/5	0.40	3.96	152,152,154,155	0
3	ADP	A	800	27/27	0.37	3.94	177,179,182,183	0
2	PO4	C	800	5/5	0.20	-0.23	151,151,152,152	0

6.5 Other polymers ⓘ

There are no such residues in this entry.