



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:14 PM GMT

PDB ID : 4BXN
Title : Eg5(WT) complex
Authors : Talapatra, S.K.; Anthony, N.G.; Mackay, S.P.; Kozielski, F.
Deposited on : 2013-07-15
Resolution : 2.79 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

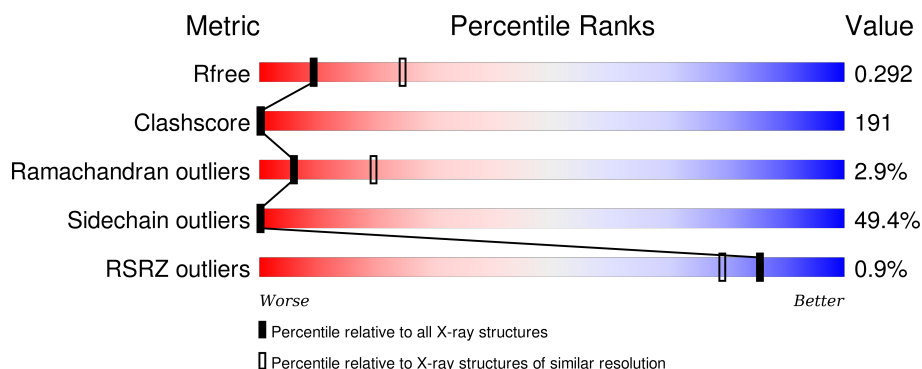
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	368	<div> <div></div> <div> <div></div> <div>12%</div> <div>44%</div> <div>38%</div> <div>• 6%</div> </div> </div>
1	B	368	<div> <div></div> <div> <div></div> <div>10%</div> <div>48%</div> <div>35%</div> <div>• 6%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	B	601	-	-	X	-
4	CL	A	1376	-	-	X	-
4	CL	A	1377	-	-	X	-
4	CL	A	1378	-	-	X	-
4	CL	A	1381	-	-	X	-
4	CL	B	1377	-	-	X	-
5	6LX	A	1375	-	-	X	-

2 Entry composition [i](#)

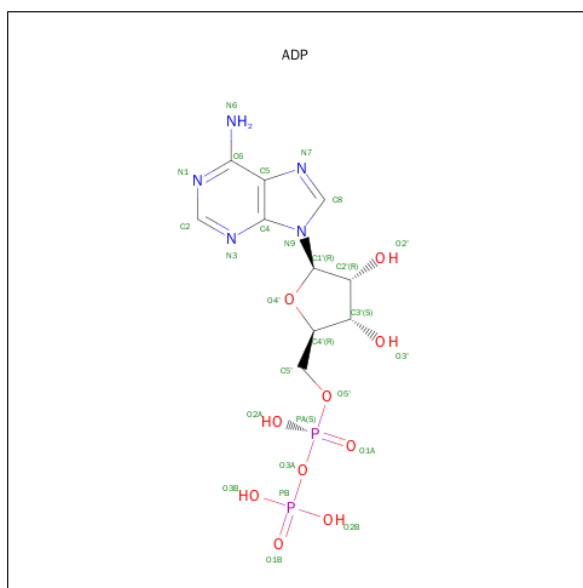
There are 6 unique types of molecules in this entry. The entry contains 5521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	2	0	0
			2663	1669	460	524	10			
1	B	345	Total	C	N	O	S	1	0	0
			2642	1657	455	520	10			

- 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		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

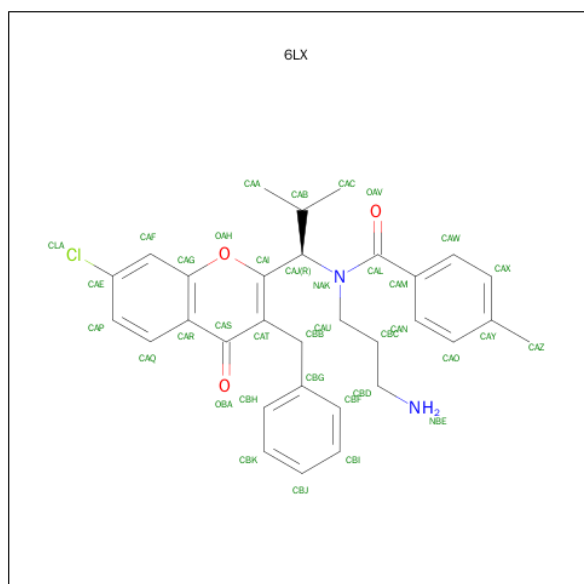
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	13	Total Cd 13 13	0	0
3	A	9	Total Cd 9 9	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total Cl 3 3	0	0
4	A	5	Total Cl 5 5	0	0

- Molecule 5 is N-(3-AMINOPROPYL)-N-[(1R)-1-(3-BENZYL-7-CHLORO-4-OXO-4H-CHROMEN-2-YL)-2-METHYLPROPYL]-4-METHYLBENZAMIDE (three-letter code: 6LX) (formula: $C_{31}H_{33}ClN_2O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 37	C 31	Cl 1	N 2	O 3	0	0
5	B	1	Total 37	C 31	Cl 1	N 2	O 3	0	0

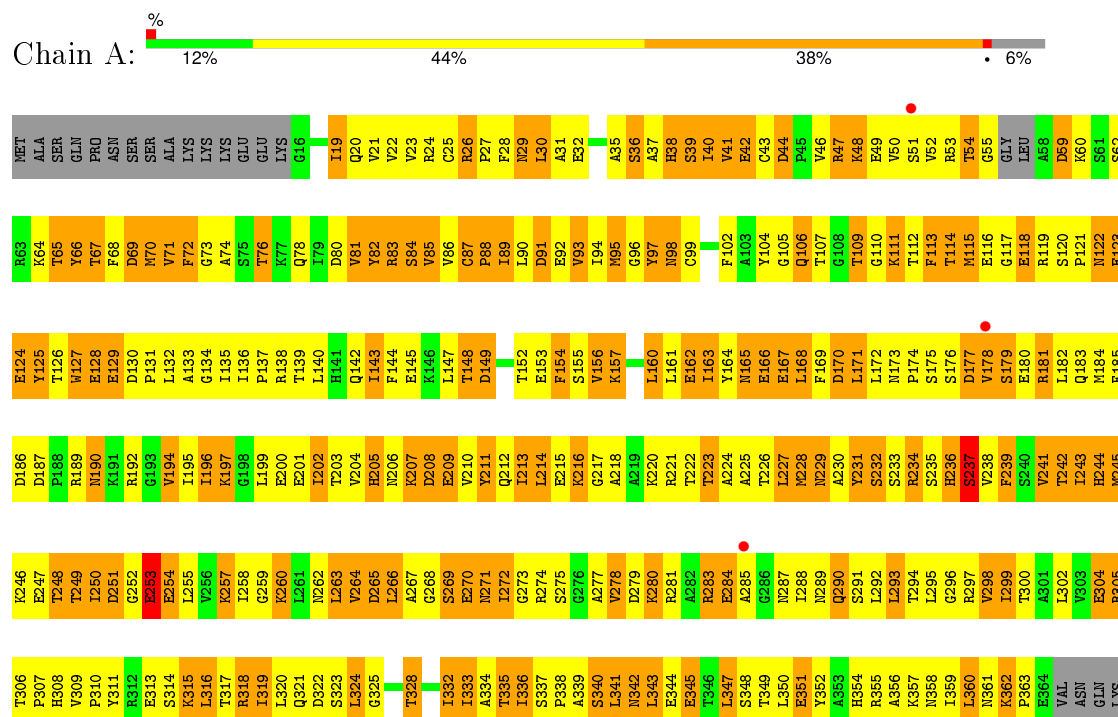
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	32	Total 32	O 32	0	0
6	B	26	Total 26	O 26	0	0

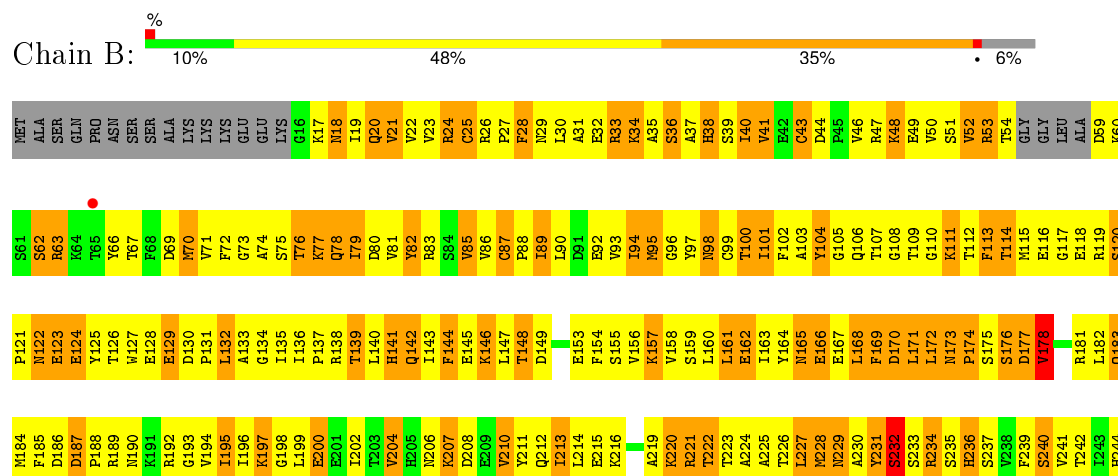
3 Residue-property plots

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: KINESIN-LIKE PROTEIN KIF11



• Molecule 1: KINESIN-LIKE PROTEIN KIF11



LYS	T306	K245
	F307	K246
	H308	E247
	Y309	T248
	P310	T249
	Y311	I250
	R312	D251
	E313	G252
	S314	E253
	K315	E254
	L316	L255
	T317	V256
	R318	K257
	I319	I258
	L320	G259
	Q321	K260
	D322	L261
	S323	N262
	L324	L263
		V264
	T328	D265
	R329	L266
	T330	A267
	S331	G268
	I332	S269
	A333	E270
	A334	N271
	T335	I272
	I336	G273
	S337	R274
	P338	S275
	A339	G276
	S340	A277
	L341	V278
	N342	D279
	L343	K280
	E344	R281
	E345	L282
	T346	R283
	L347	E284
	S348	A285
	T349	G286
	L350	N287
	E351	I288
	Y352	
	A353	S291
	H354	L292
	R355	L293
	A356	T294
	K357	L295
	N358	G296
	I359	R297
	L360	V298
	N361	I299
	K362	T300
	P363	A301
	E364	L302
	VAL	V303
	ASN	E304
	GLN	R305

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.43Å 81.43Å 115.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.93 – 2.79 27.94 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.1 (27.93-2.79) 97.1 (27.94-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.80Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.274 0.280 , 0.292	Depositor DCC
R_{free} test set	1059 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 54.8	EDS
Estimated twinning fraction	0.500 for -H,-K,L 0.477 for -h,-k,l 0.075 for h,-h-k,-l 0.070 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -H,-K,L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 20599 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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: 6LX, CL, ADP, CD

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	0.31	0/2702	0.46	0/3658
1	B	0.31	0/2680	0.58	2/3630 (0.1%)
All	All	0.31	0/5382	0.52	2/7288 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	173	ASN	C-N-CD	-18.59	79.70	120.60
1	B	309	VAL	C-N-CD	-5.21	109.13	120.60

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	2663	0	2620	1035	17
1	B	2642	0	2599	1009	24
2	A	27	0	12	3	0
2	B	27	0	12	21	0
3	A	9	0	0	1	0
3	B	13	0	0	1	1
4	A	5	0	0	10	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	3	0
5	A	37	0	33	89	0
5	B	37	0	33	9	0
6	A	32	0	0	12	0
6	B	26	0	0	4	0
All	All	5521	0	5309	2057	30

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 191.

The worst 5 of 2057 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:72:PHE:CE2	1:A:81:VAL:HG22	1.21	1.63
1:A:28:PHE:CE1	1:A:339:ALA:CB	1.80	1.63
1:A:28:PHE:CZ	1:A:339:ALA:CB	1.77	1.62
1:A:211:TYR:CE1	5:A:1375:6LX:HAA1	1.34	1.60
1:B:113:PHE:CE2	1:B:118:GLU:HG3	1.26	1.60

The worst 5 of 30 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:NH2	1:B:253:GLU:CD[3_565]	0.48	1.72
1:A:59:ASP:OD2	1:A:287:ASN:ND2[3_565]	0.80	1.40
1:B:33:ARG:CZ	1:B:253:GLU:OE1[3_565]	0.90	1.30
1:A:344:GLU:OE2	3:B:1369:CD:CD[3_565]	1.04	1.16
1:B:33:ARG:NH2	1:B:253:GLU:CG[3_565]	1.07	1.13

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	343/368 (93%)	325 (95%)	9 (3%)	9 (3%)	7	22
1	B	341/368 (93%)	318 (93%)	12 (4%)	11 (3%)	5	17
All	All	684/736 (93%)	643 (94%)	21 (3%)	20 (3%)	6	19

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	179	SER
1	B	18	ASN
1	B	53	ARG
1	B	74	ALA

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	290/322 (90%)	141 (49%)	149 (51%)	0	0
1	B	287/322 (89%)	151 (53%)	136 (47%)	0	0
All	All	577/644 (90%)	292 (51%)	285 (49%)	0	0

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	LYS
1	B	41	VAL
1	B	315	LYS
1	A	324	LEU
1	A	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	20	GLN
1	B	212	GLN
1	A	290	GLN
1	B	183	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 34 ligands modelled in this entry, 30 are monoatomic - leaving 4 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	$\# Z > 2$
5	6LX	A	1375	-	38,40,40	2.47	15 (39%)	44,56,56	1.42	7 (15%)
2	ADP	A	601	3	22,29,29	0.94	1 (4%)	27,45,45	2.14	5 (18%)
5	6LX	B	1375	-	38,40,40	2.14	10 (26%)	44,56,56	1.93	9 (20%)
2	ADP	B	601	3	22,29,29	1.01	1 (4%)	27,45,45	1.94	4 (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
5	6LX	A	1375	-	-	0/24/28/28	0/4/4/4
2	ADP	A	601	3	-	0/12/32/32	0/3/3/3
5	6LX	B	1375	-	-	0/24/28/28	0/4/4/4
2	ADP	B	601	3	-	0/12/32/32	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1375	6LX	OAH-CAI	-3.80	1.30	1.35
5	A	1375	6LX	OAH-CAI	-2.76	1.31	1.35
5	A	1375	6LX	CAB-CAJ	-2.27	1.48	1.54
5	A	1375	6LX	CAQ-CAP	2.12	1.41	1.36
5	B	1375	6LX	CBJ-CBK	2.14	1.43	1.38

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ADP	N3-C2-N1	-7.83	122.90	128.89
2	B	601	ADP	N3-C2-N1	-6.73	123.74	128.89
5	B	1375	6LX	CAT-CBB-CBG	-3.75	105.04	113.64
2	B	601	ADP	PA-O3A-PB	-3.64	120.47	132.67
2	A	601	ADP	C4-C5-N7	-3.64	106.14	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 122 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1375	6LX	89	0
2	A	601	ADP	3	0
5	B	1375	6LX	9	0
2	B	601	ADP	21	0

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 [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	347/368 (94%)	-0.02	3 (0%)	85 79	49, 71, 88, 93	1 (0%)
1	B	345/368 (93%)	-0.05	3 (0%)	85 79	48, 72, 87, 96	0
All	All	692/736 (94%)	-0.04	6 (0%)	85 79	48, 72, 88, 96	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	ALA	3.2
1	B	285	ALA	3.0
1	A	178	VAL	2.8
1	B	364	GLU	2.8
1	B	65	THR	2.7

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(\AA^2)	Q<0.9
5	6LX	A	1375	37/37	0.78	0.21	1.33	67,76,80,87	0
5	6LX	B	1375	37/37	0.85	0.21	0.52	67,76,80,87	0
4	CL	A	1374	1/1	0.96	0.13	-0.40	54,54,54,54	0
2	ADP	B	601	27/27	0.94	0.14	-0.41	60,67,69,73	0
3	CD	A	1367	1/1	0.98	0.10	-1.05	59,59,59,59	0
3	CD	B	1370	1/1	0.99	0.14	-1.13	60,60,60,60	0
4	CL	A	1377	1/1	0.98	0.09	-1.15	74,74,74,74	0
2	ADP	A	601	27/27	0.90	0.12	-1.29	61,66,74,79	0
4	CL	A	1376	1/1	0.85	0.13	-1.31	85,85,85,85	0
3	CD	B	1374	1/1	0.98	0.09	-1.38	115,115,115,115	0
3	CD	A	1368	1/1	0.97	0.11	-1.44	91,91,91,91	0
3	CD	B	1368	1/1	0.99	0.08	-1.49	51,51,51,51	0
3	CD	A	1371	1/1	0.98	0.07	-1.96	100,100,100,100	0
3	CD	A	1370	1/1	0.99	0.08	-2.08	69,69,69,69	0
3	CD	A	1365	1/1	0.97	0.12	-2.12	66,66,66,66	0
4	CL	A	1378	1/1	0.89	0.11	-2.19	84,84,84,84	0
3	CD	B	1365	1/1	0.98	0.06	-2.19	82,82,82,82	0
3	CD	B	1369	1/1	0.96	0.10	-2.20	80,80,80,80	0
3	CD	A	1369	1/1	0.98	0.07	-2.63	100,100,100,100	0
3	CD	B	1378	1/1	0.90	0.03	-2.79	106,106,106,106	0
3	CD	B	1367	1/1	0.98	0.04	-3.03	78,78,78,78	0
3	CD	B	1376	1/1	0.98	0.06	-	30,30,30,30	0
4	CL	B	1385	1/1	0.82	0.17	-	83,83,83,83	0
3	CD	A	1372	1/1	0.94	0.14	-	104,104,104,104	0
3	CD	B	1379	1/1	0.93	0.04	-	120,120,120,120	0
3	CD	B	1366	1/1	0.97	0.07	-	90,90,90,90	0
3	CD	A	1373	1/1	0.98	0.07	-	112,112,112,112	0
3	CD	B	1372	1/1	0.96	0.04	-	115,115,115,115	0
3	CD	B	1373	1/1	0.98	0.04	-	107,107,107,107	0
4	CL	A	1381	1/1	0.91	0.07	-	80,80,80,80	0
3	CD	A	1366	1/1	0.96	0.04	-	86,86,86,86	0
4	CL	B	1386	1/1	0.98	0.19	-	66,66,66,66	0
4	CL	B	1377	1/1	0.94	0.08	-	67,67,67,67	0
3	CD	B	1371	1/1	0.99	0.02	-	100,100,100,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.