



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:47 AM GMT

PDB ID : 3C7N
Title : Structure of the Hsp110:Hsc70 Nucleotide Exchange Complex
Authors : Schuermann, J.P.; Jiang, J.; Hart, P.J.; Sousa, R.
Deposited on : 2008-02-07
Resolution : 3.12 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

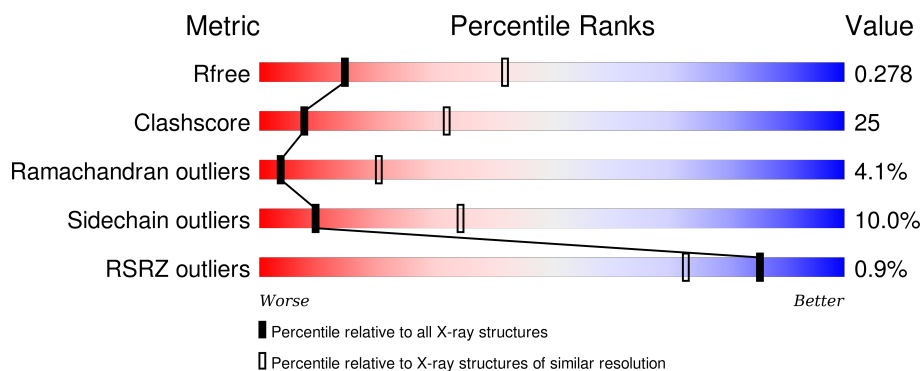
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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	668	<div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> <div>.</div> </div>
2	B	554	<div> <div></div> <div>49%</div> <div>40%</div> <div>9%</div> <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
3	MG	A	667	-	-	-	X
4	CL	B	555	-	-	X	-
5	SO4	A	668	-	-	-	X
5	SO4	A	669	-	-	-	X
5	SO4	A	670	-	-	-	X
6	BEF	A	671	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9368 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 Heat shock protein homolog SSE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5103	3227	853	1010	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P32589
A	0	PRO	-	EXPRESSION TAG	UNP P32589

- Molecule 2 is a protein called Heat shock cognate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	540	Total	C	N	O	S	0	0	0
			4182	2621	726	824	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

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

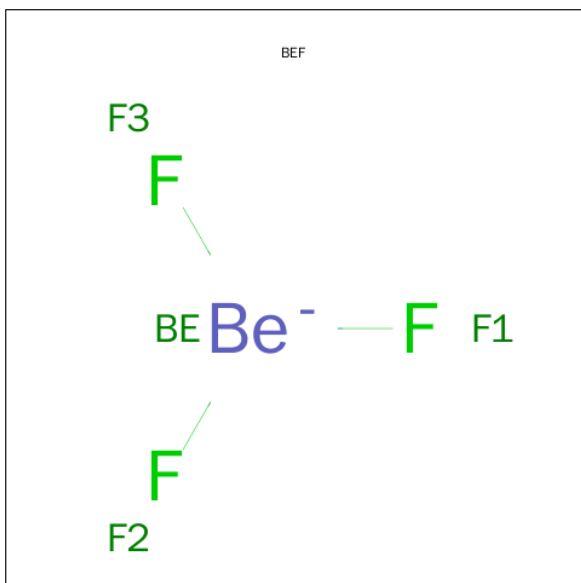
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



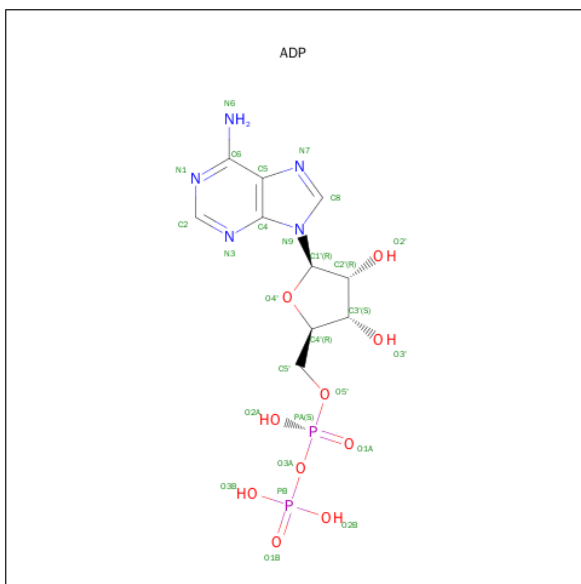
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Be	F	0	0
			4	1	3		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

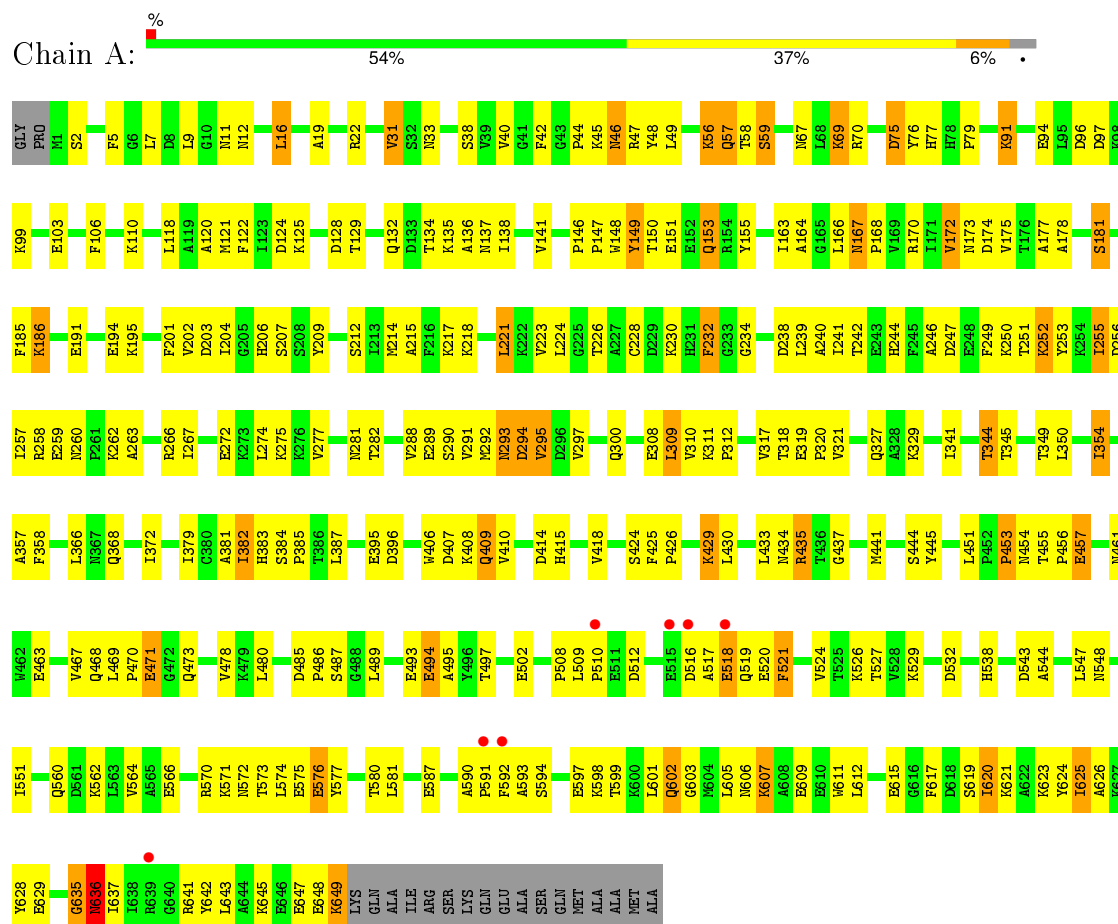


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

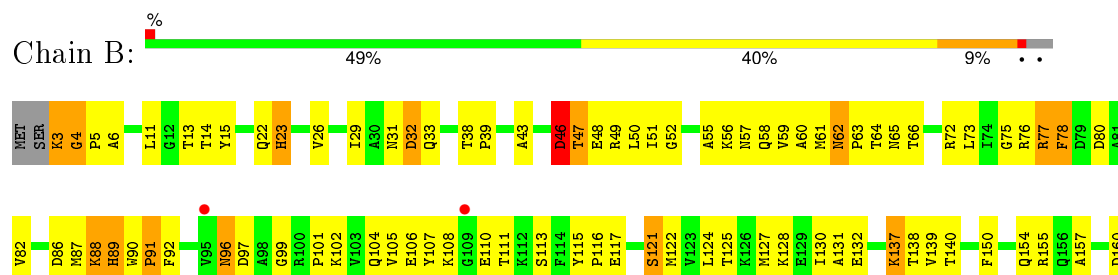
3 Residue-property plots

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: Heat shock protein homolog SSE1



• Molecule 2: Heat shock cognate



T502	I503	T504	N505	D506	K507	G508	A509	L510	S511	T512	K513	E514	D515		R517		K526	E528	D529	E530	K531	Q532		K535		S538	K539	N540	S541	L542	E543	S544	Y545	A546	F547	ASN	MET	LYS	ALA	THR	VAL	GLU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
V409	T419	I420	P421	T425		F428	T429	G430	T430	Y431	S432	D433	T434	Q435	P436	Q437	V438	L439	V442	R447	A448	M449	T450	K451	D452		F459	E460	L461	T462	G463	I464	A467	P468	R469	G470	V471	P472		T477		I480		L485		V488		V491		T495	G496	K497	K500	I501																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
K328	S329	Q330		D333		L336	G337	G338	G339	S340	T341	R342	I343	F344	K345	I346		Q351	R352	F353	F354	N355		L359	R360	K361		N364	P365		A368		Y371	G372		V375	Q376	A377	A378		D383	K384	SER	GLU	ASN	VAL	GLN		D390	L391	L392	L393	L394	D395		I403	E404	T405	A406																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
H249	K250	K251	D252	I253	S254	E255	N256	K257	R258	A259	V260	R261		C267	E268		K271	R272		T278	Q279	A280		E283	L284	D285	I286		I291	D292		T295	S296	I297	T298	R299	A300	R301	F302	E303	E304	L305	N306		I309	F310		L314	D315	P316		K319	A320	I242	A243	E244	F245	K246	R247	K248																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																														
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.53Å 169.50Å 87.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 3.12 42.38 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.38-3.12) 96.6 (42.38-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.283 0.221 , 0.278	Depositor DCC
R_{free} test set	1652 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 32506 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9368	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: MG, BEF, SO4, ADP, CL

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	0.56	0/5199	0.70	0/7037
2	B	0.56	1/4242 (0.0%)	0.70	1/5728 (0.0%)
All	All	0.56	1/9441 (0.0%)	0.70	1/12765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ARG	CG-CD	5.82	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	420	ILE	Peptide

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	5103	0	5079	245	0
2	B	4182	0	4209	243	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	B	3	0	0	2	0
5	A	15	0	0	0	0
5	B	5	0	0	0	0
6	A	4	0	0	0	0
7	A	27	0	12	1	0
7	B	27	0	12	5	0
All	All	9368	0	9312	473	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 25.

The worst 5 of 473 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)
2:B:420:ILE:HG23	2:B:421:PRO:CD	1.75	1.15
1:A:594:SER:HB3	1:A:597:GLU:HG2	1.32	1.11
1:A:601:LEU:O	1:A:603:GLY:HA3	1.53	1.09
1:A:141:VAL:HG21	1:A:166:LEU:HD13	1.40	1.03
2:B:405:THR:HB	2:B:409:VAL:HG23	1.44	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	647/668 (97%)	546 (84%)	80 (12%)	21 (3%)	5	27
2	B	536/554 (97%)	442 (82%)	67 (12%)	27 (5%)	3	16
All	All	1183/1222 (97%)	988 (84%)	147 (12%)	48 (4%)	3	20

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	457	GLU
1	A	471	GLU
1	A	636	ASN
1	A	637	ILE

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	560/573 (98%)	511 (91%)	49 (9%)	12	43
2	B	455/468 (97%)	403 (89%)	52 (11%)	7	28
All	All	1015/1041 (98%)	914 (90%)	101 (10%)	9	34

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	620	ILE
2	B	77	ARG
2	B	504	THR
1	A	636	ASN
2	B	14	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	ASN
1	A	572	ASN
2	B	376	GLN
1	A	519	GLN
1	A	606	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	SO4	A	668	-	4,4,4	0.15	0	6,6,6	0.15	0
5	SO4	A	669	-	4,4,4	0.20	0	6,6,6	0.43	0
5	SO4	A	670	-	4,4,4	0.39	0	6,6,6	0.45	0
6	BEF	A	671	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	A	672	3,6	22,29,29	1.04	1 (4%)	27,45,45	2.03	5 (18%)
5	SO4	B	559	-	4,4,4	0.19	0	6,6,6	0.26	0
7	ADP	B	560	-	22,29,29	0.99	1 (4%)	27,45,45	2.41	8 (29%)

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	SO4	A	668	-	-	0/0/0/0	0/0/0/0
5	SO4	A	669	-	-	0/0/0/0	0/0/0/0
5	SO4	A	670	-	-	0/0/0/0	0/0/0/0
6	BEF	A	671	7	-	0/0/0/0	0/0/0/0
7	ADP	A	672	3,6	-	0/12/32/32	0/3/3/3
5	SO4	B	559	-	-	0/0/0/0	0/0/0/0
7	ADP	B	560	-	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	560	ADP	C5-C4	2.99	1.47	1.40
7	A	672	ADP	C5-C4	3.34	1.48	1.40

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	560	ADP	N3-C2-N1	-8.03	122.74	128.89
7	A	672	ADP	N3-C2-N1	-6.44	123.96	128.89
7	B	560	ADP	C4-C5-N7	-4.99	104.89	109.48
7	A	672	ADP	C2'-C1'-N9	-4.52	107.39	114.29
7	B	560	ADP	PA-O3A-PB	-3.37	121.36	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	672	ADP	1	0
7	B	560	ADP	5	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	649/668 (97%)	-0.26	7 (1%) 82 67	10, 42, 114, 147	0
2	B	540/554 (97%)	-0.21	4 (0%) 89 79	22, 50, 99, 136	0
All	All	1189/1222 (97%)	-0.24	11 (0%) 85 73	10, 47, 107, 147	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	508	GLY	3.6
1	A	591	PRO	3.0
1	A	516	ASP	2.8
2	B	109	GLY	2.6
2	B	383	ASP	2.4

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(\AA^2)	Q<0.9
5	SO4	A	669	5/5	0.91	0.33	12.00	76,79,80,82	0
3	MG	A	667	1/1	0.97	0.41	9.79	14,14,14,14	0
6	BEF	A	671	4/4	0.97	0.34	6.12	39,39,39,39	0
5	SO4	A	670	5/5	0.87	0.28	4.10	103,106,108,109	0
5	SO4	A	668	5/5	0.97	0.34	3.86	81,83,85,86	0
4	CL	B	556	1/1	0.86	0.22	1.36	65,65,65,65	0
7	ADP	B	560	27/27	0.93	0.23	1.31	60,60,60,60	0
7	ADP	A	672	27/27	0.96	0.23	1.13	44,44,44,44	0
5	SO4	B	559	5/5	0.96	0.24	0.95	70,72,74,75	0
4	CL	B	555	1/1	0.85	0.15	-1.68	69,69,69,69	0
4	CL	B	557	1/1	0.97	0.15	-	48,48,48,48	0
3	MG	B	558	1/1	0.94	0.34	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.