



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:32 PM GMT

PDB ID : 3C7N
Title : Structure of the Hsp110:Hsc70 Nucleotide Exchange Complex
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Deposited on : 2008-02-07
Resolution : 3.12 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>

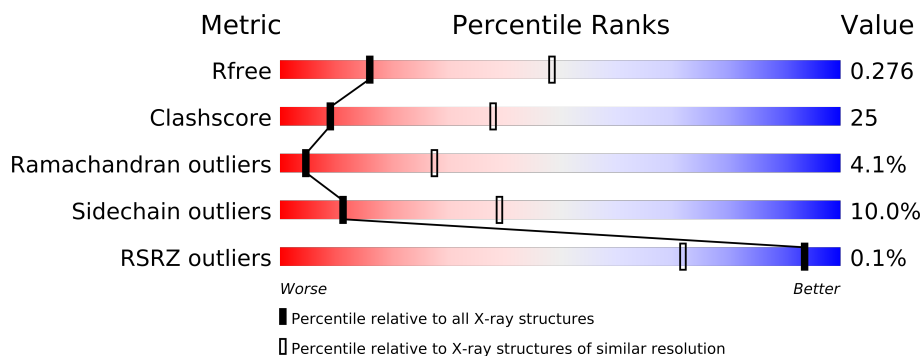
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.12 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}	66092	1466 (3.20-3.04)
Clashscore	79885	1067 (3.18-3.06)
Ramachandran outliers	78287	1034 (3.18-3.06)
Sidechain outliers	78261	1034 (3.18-3.06)
RSRZ outliers	66119	1468 (3.20-3.04)

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	668	
2	B	554	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	667	-	X
3	MG	B	558	-	X
5	SO4	A	668	-	X
5	SO4	A	669	-	X
5	SO4	A	670	-	X
6	BEF	A	671	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9368 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 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).

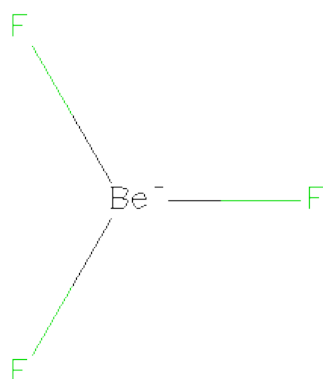
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Cl	0	0
			3	3		

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



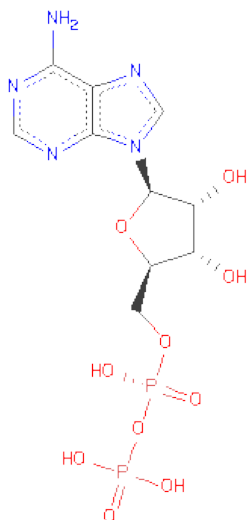
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- 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: $C_{10}H_{15}N_5O_{10}P_2$).



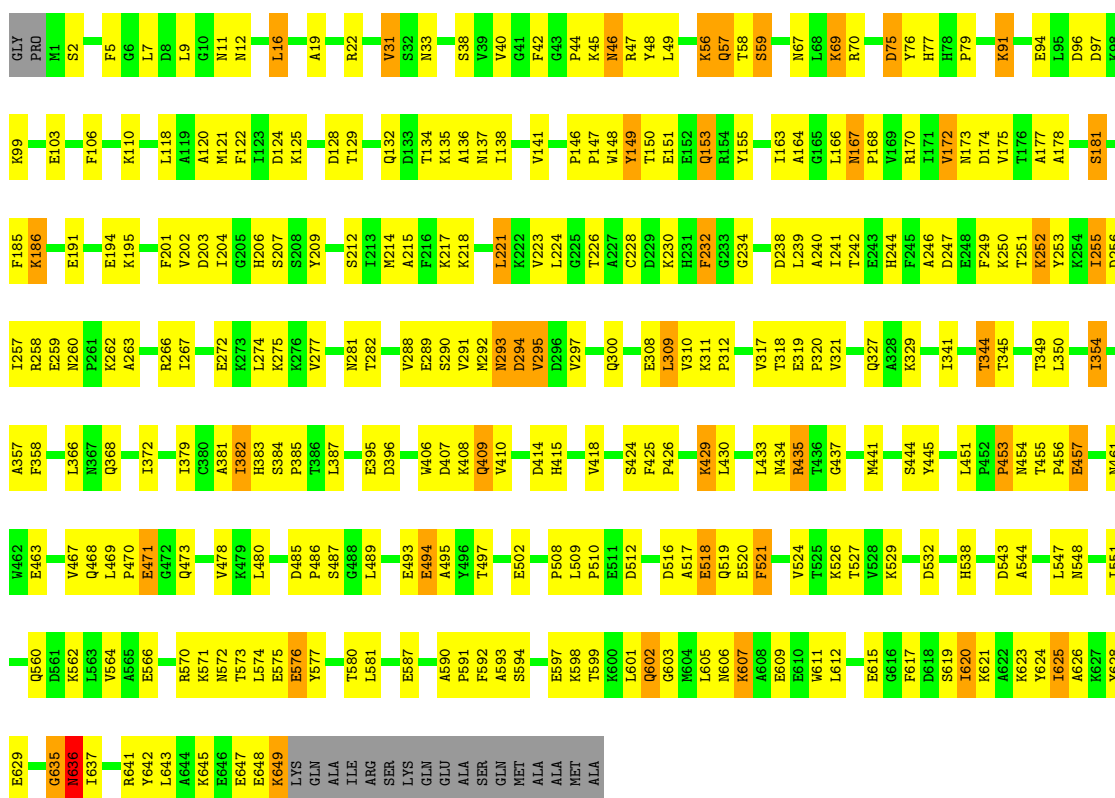
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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.

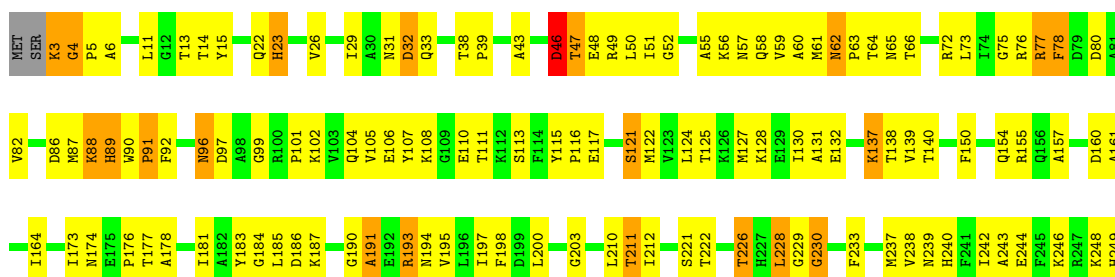
- Molecule 1: Heat shock protein homolog SSE1

Chain A:



- Molecule 2: Heat shock cognate

Chain B:



T504	K250	S329	T419	T504
N505	K251	Q330	T420	N505
D506	D252	D333	P421	D506
K507	T253			K507
G508	S254	L336	T425	G508
R509	E255	Y337		R509
L510	I256	G338	F428	L510
S511	K257	G339	T429	S511
K512	A258	R259	T430	K512
E513	A259	S340	Y431	E513
D514	V260	T341	S432	D514
	R261	R342	D433	
R517		I343	V434	R517
	C267	F344	Q435	
K526	E268	K345	P436	K526
A527		I346	G437	A527
E528	K271		Y438	E528
D529	R272	Q351	L439	D529
E530		D352		E530
K531	T278	F353	V442	K531
Q532	Q279	N355		Q532
K535	A280		R447	K535
			A448	
S538	E283	L359	N449	S538
K539	T284	N360	T450	K539
N540	D285	K361	K451	N540
S541	S286		D452	S541
L542	T291	N364	F459	L542
E543	D292	P365	E460	E543
S544	T295		L461	S544
Y545	S296	A368	T462	Y545
A546	T297	Y371	G463	A546
F547	T298	G372	T464	F547
ASN	T299			ASN
MEI	A300	V375	A467	MEI
LYS	R301	Q376	P468	LYS
ALA	F302	A377	R469	ALA
THR	E303	A378	G470	THR
VAL	E304		V471	VAL
GLU	L305	K384	P472	GLU
	N306	SER		
		GLU	T477	
	L309	ASN		
	F310	VAL	T480	
		GLN		
	L314	D390	T485	
	D315	L391		
	P316	L392	V488	
		L393		
	K319	L394	V491	
	A320	D395		
	L321		T495	
		I403	G496	
	A324	E404	K497	
	K325	T405		
	L326	A406	K500	
	D327		I501	
	K328	V409	T502	
			I503	

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 0.216 , 0.276	Depositor DCC
R_{free} test set	1650 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 10.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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.

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 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	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

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 25.

The worst 5 of 473 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	647/668 (97%)	546 (84%)	80 (12%)	21 (3%)	6	35
2	B	536/554 (97%)	442 (82%)	67 (12%)	27 (5%)	3	22
All	All	1183/1222 (97%)	988 (84%)	147 (12%)	48 (4%)	4	27

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%)	14	50
2	B	455/468 (97%)	403 (89%)	52 (11%)	8	32
All	All	1015/1041 (98%)	914 (90%)	101 (10%)	11	39

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

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Mol	Chain	Res	Type
1	A	519	GLN
1	A	606	ASN

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 ⓘ

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	0.13	0	6,6,6	0.15	0
5	SO4	A	669	-	4,4,4	0.19	0	6,6,6	0.41	0
5	SO4	A	670	-	4,4,4	0.42	0	6,6,6	0.43	0
6	BEF	A	671	7	0,3,3	0.00	-	0,3,3	0.00	-
7	ADP	A	672	3,6	29,29,29	1.08	2 (6%)	45,45,45	2.00	9 (20%)
5	SO4	B	559	-	4,4,4	0.17	0	6,6,6	0.25	0
7	ADP	B	560	-	29,29,29	1.26	4 (13%)	45,45,45	2.19	12 (26%)

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	-	0/16/32/32	0/1/3/3
5	SO4	B	559	-	-	0/0/0/0	0/0/0/0
7	ADP	B	560	-	-	0/16/32/32	0/1/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	672	ADP	C5-C4	3.34	1.48	1.40
7	B	560	ADP	C4-N9	-3.28	1.33	1.37
7	B	560	ADP	C5-C4	2.99	1.47	1.40
7	A	672	ADP	C4-N9	-2.61	1.33	1.37
7	B	560	ADP	PB-O3A	2.11	1.63	1.60

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	560	ADP	N3-C2-N1	-7.14	122.74	128.71
7	A	672	ADP	O4'-C1'-N9	6.75	114.72	108.44
7	A	672	ADP	N3-C2-N1	-5.68	123.96	128.71
7	B	560	ADP	C4-C5-N7	-5.40	104.89	109.52
7	A	672	ADP	N3-C4-N9	5.11	134.66	125.43

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	649/668 (97%)	-0.23	0 100 100	10, 42, 114, 147	0
2	B	540/554 (97%)	-0.19	0 100 100	22, 50, 99, 136	0
All	All	1189/1222 (97%)	-0.21	0 93 100	10, 47, 107, 147	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	MG	A	667	1/1	0.40	12.11	14,14,14,14	0
5	SO4	A	669	5/5	0.31	11.58	76,79,80,82	0
6	BEF	A	671	4/4	0.34	6.67	39,39,39,39	0
3	MG	B	558	1/1	0.30	5.17	27,27,27,27	0
5	SO4	A	670	5/5	0.24	3.87	103,106,108,109	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	668	5/5	0.32	3.07	81,83,85,86	0
4	CL	B	556	1/1	0.20	1.61	65,65,65,65	0
7	ADP	A	672	27/27	0.24	1.50	44,44,44,44	0
7	ADP	B	560	27/27	0.23	1.48	60,60,60,60	0
4	CL	B	557	1/1	0.17	0.57	48,48,48,48	0
5	SO4	B	559	5/5	0.21	0.12	70,72,74,75	0
4	CL	B	555	1/1	0.12	-1.73	69,69,69,69	0

6.5 Other polymers ⓘ

There are no such residues in this entry.