



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:50 PM GMT

PDB ID : 4JNE  
Title : Allosteric opening of the polypeptide-binding site when an Hsp70 binds ATP  
Authors : Qi, R.; Sarbeng, E.B.; Liu, Q.; Le, K.Q.; Xu, X.; Xu, H.; Yang, J.; Wong, J.L.;  
Vorvis, C.; Hendrickson, W.A.; Zhou, L.; Liu, Q.  
Deposited on : 2013-03-15  
Resolution : 1.96 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](mailto: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.

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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

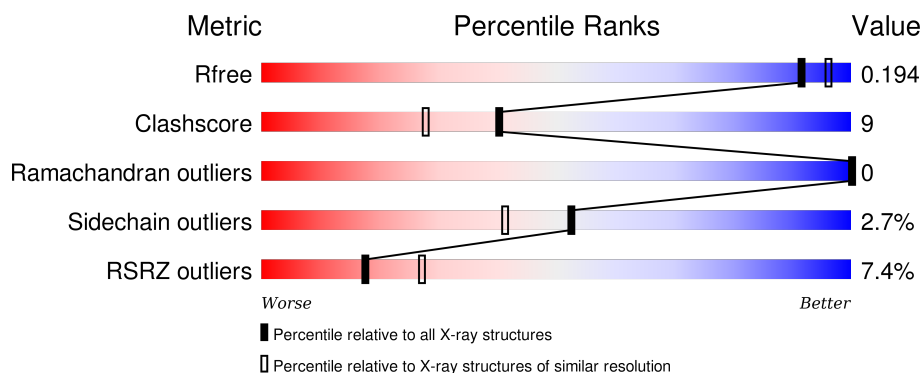
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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  $\geq 3$ , 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	608	<div> <div>7%</div> <div>83%</div> <div>15%</div> <div>..</div> </div>
1	B	608	<div> <div>8%</div> <div>83%</div> <div>15%</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
4	SO4	A	1006	-	-	-	X
4	SO4	A	1007	-	-	-	X
4	SO4	B	1006	-	-	-	X
4	SO4	B	1007	-	-	-	X
5	GOL	A	1008	-	-	-	X
5	GOL	A	1009	-	-	-	X
5	GOL	B	1010	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10677 atoms, of which 32 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 Hsp70 CHAPERONE DnaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	600	Total	C	N	O	S	0	0	0
			4550	2828	791	915	16			
1	B	600	Total	C	N	O	S	0	0	0
			4550	2828	791	915	16			

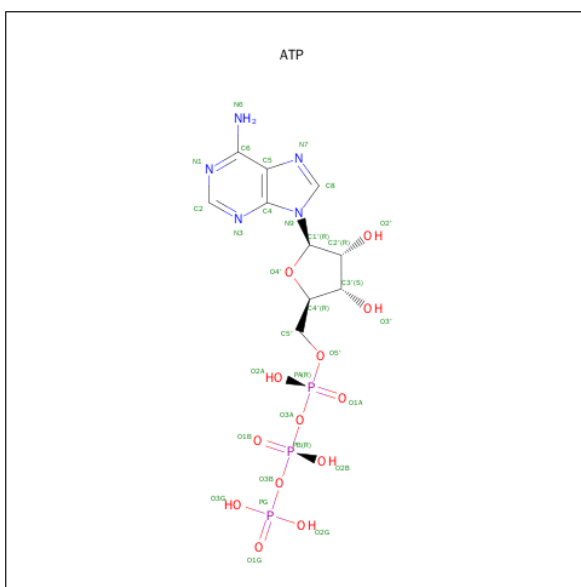
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP P0A6Y8
A	199	ALA	THR	CONFLICT	UNP P0A6Y8
A	?	-	THR	DELETION	UNP P0A6Y8
A	?	-	ALA	DELETION	UNP P0A6Y8
A	?	-	GLU	DELETION	UNP P0A6Y8
A	?	-	ASP	DELETION	UNP P0A6Y8
A	428	MET	ASN	ENGINEERED MUTATION	UNP P0A6Y8
A	429	GLY	GLN	ENGINEERED MUTATION	UNP P0A6Y8
A	430	GLY	SER	ENGINEERED MUTATION	UNP P0A6Y8
A	611	HIS	-	EXPRESSION TAG	UNP P0A6Y8
A	612	ALA	-	EXPRESSION TAG	UNP P0A6Y8
B	1	SER	-	EXPRESSION TAG	UNP P0A6Y8
B	199	ALA	THR	CONFLICT	UNP P0A6Y8
B	?	-	THR	DELETION	UNP P0A6Y8
B	?	-	ALA	DELETION	UNP P0A6Y8
B	?	-	GLU	DELETION	UNP P0A6Y8
B	?	-	ASP	DELETION	UNP P0A6Y8
B	428	MET	ASN	ENGINEERED MUTATION	UNP P0A6Y8
B	429	GLY	GLN	ENGINEERED MUTATION	UNP P0A6Y8
B	430	GLY	SER	ENGINEERED MUTATION	UNP P0A6Y8
B	611	HIS	-	EXPRESSION TAG	UNP P0A6Y8
B	612	ALA	-	EXPRESSION TAG	UNP P0A6Y8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	1
			10	8	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

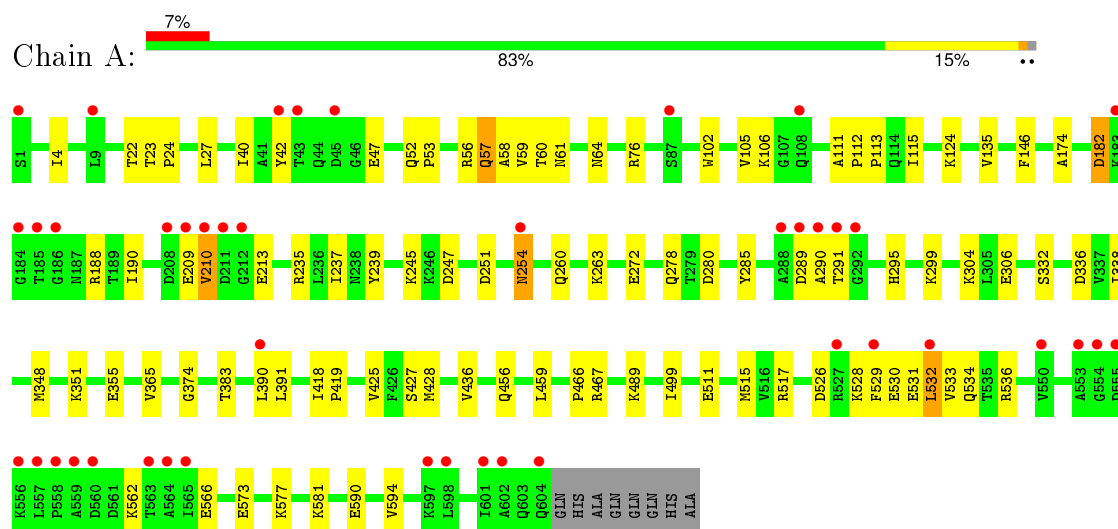
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	680	Total	O	0	0
			680	680		
6	B	717	Total	O	0	0
			717	717		

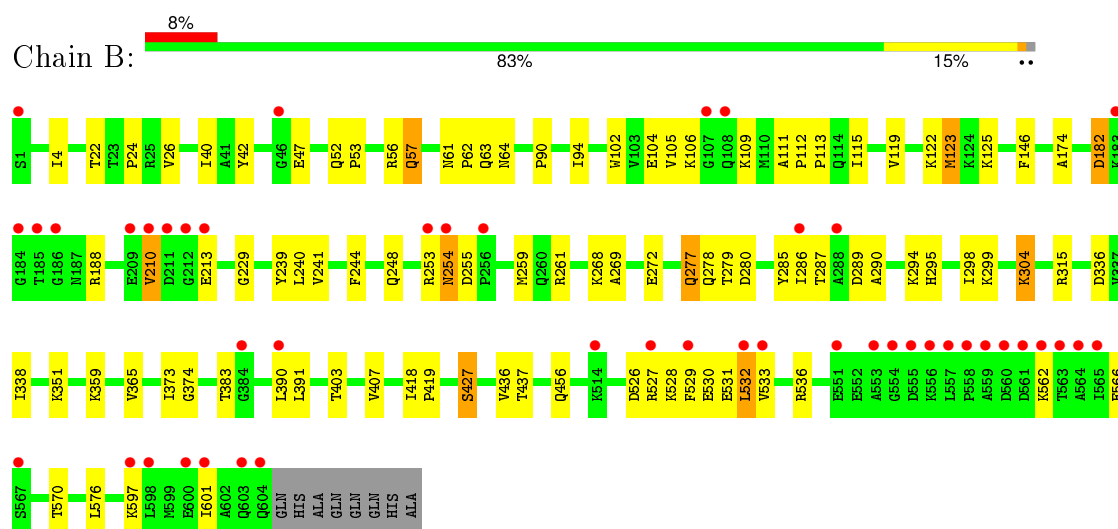
### 3 Residue-property plots [i](#)

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: Hsp70 CHAPERONE DnaK



#### • Molecule 1: Hsp70 CHAPERONE DnaK





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	290.68Å 290.68Å 99.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 1.96 38.31 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.97-1.96) 99.8 (38.31-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 1.97Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.173 , 0.201 0.165 , 0.194	Depositor DCC
$R_{free}$ test set	7536 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 150466 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10677	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, MG, SO4, ATP

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	0.28	0/4602	0.45	0/6217
1	B	0.29	0/4602	0.46	0/6217
All	All	0.28	0/9204	0.46	0/12434

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	4550	0	4610	75	0
1	B	4550	0	4610	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	1	0
4	A	25	0	0	0	0
4	B	35	0	0	0	0
5	A	12	16	16	3	0
5	B	12	16	16	2	0
6	A	680	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	717	0	0	16	0
All	All	10645	32	9276	161	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 9.

All (161) 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:B:123:MET:HA	1:B:123:MET:HE2	1.24	1.17
1:A:285:TYR:H	1:A:295:HIS:HD2	1.08	1.00
1:B:42:TYR:HD2	1:B:105:VAL:HG11	1.36	0.91
1:B:123:MET:SD	6:B:1210:HOH:O	2.28	0.90
1:B:531:GLU:HG3	6:B:1573:HOH:O	1.71	0.89
1:B:123:MET:HA	1:B:123:MET:CE	2.04	0.87
1:B:280:ASP:OD1	1:B:299:LYS:HG2	1.78	0.83
1:B:123:MET:HE2	1:B:123:MET:CA	2.06	0.82
1:A:285:TYR:H	1:A:295:HIS:CD2	1.94	0.82
1:A:42:TYR:HD2	1:A:105:VAL:HG11	1.43	0.80
1:A:534:GLN:HG3	6:A:1699:HOH:O	1.82	0.80
1:B:63:GLN:HA	6:B:1737:HOH:O	1.85	0.76
1:B:123:MET:CE	1:B:123:MET:CA	2.64	0.74
1:B:255:ASP:O	1:B:259:MET:HG2	1.88	0.74
1:B:64:ASN:HD22	1:B:106:LYS:HE2	1.53	0.72
1:B:285:TYR:H	1:B:295:HIS:HD2	1.37	0.72
1:B:285:TYR:H	1:B:295:HIS:CD2	2.07	0.72
1:A:57:GLN:HE22	1:A:61:ASN:HD22	1.37	0.71
1:A:280:ASP:OD1	1:A:299:LYS:HG2	1.90	0.70
1:B:390:LEU:HD23	1:B:391:LEU:N	2.06	0.70
1:A:278:GLN:OE1	1:B:536:ARG:HD2	1.90	0.70
1:B:289:ASP:OD1	1:B:290:ALA:N	2.29	0.66
1:A:285:TYR:N	1:A:295:HIS:HD2	1.88	0.66
1:B:64:ASN:ND2	1:B:106:LYS:HE2	2.12	0.65
1:A:245:LYS:NZ	1:A:251:ASP:HB2	2.12	0.64
1:B:42:TYR:CD2	1:B:105:VAL:HG11	2.25	0.64
1:A:64:ASN:HD22	1:A:106:LYS:HE2	1.61	0.64
1:B:57:GLN:HE22	1:B:61:ASN:HD22	1.45	0.63
1:B:562:LYS:O	1:B:566:GLU:HG3	1.97	0.63
1:B:531:GLU:N	6:B:1573:HOH:O	2.22	0.62
1:B:123:MET:HE3	1:B:123:MET:N	2.14	0.62
1:A:27:LEU:HA	5:A:1008:GOL:H12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD11	1:B:119:VAL:HG23	1.81	0.61
1:A:64:ASN:ND2	1:A:106:LYS:HE2	2.15	0.61
1:A:526:ASP:O	1:A:530:GLU:HG3	2.01	0.61
1:A:190:ILE:HG22	1:A:336:ASP:HB2	1.83	0.60
1:B:40:ILE:HD12	1:B:40:ILE:N	2.17	0.60
1:A:390:LEU:HD23	1:A:391:LEU:N	2.17	0.59
1:A:511:GLU:O	1:A:515:MET:HG3	2.02	0.59
1:B:4:ILE:HD12	1:B:383:THR:HG23	1.86	0.58
1:B:94:ILE:HD13	1:B:104:GLU:HB2	1.86	0.57
1:A:562:LYS:O	1:A:566:GLU:HG3	2.03	0.57
6:A:1753:HOH:O	1:B:299:LYS:HE2	2.05	0.57
1:B:188:ARG:HD3	1:B:336:ASP:OD2	2.05	0.56
1:B:123:MET:N	1:B:123:MET:CE	2.69	0.56
1:A:40:ILE:HD12	1:A:40:ILE:N	2.20	0.56
1:A:304:LYS:HE3	1:A:304:LYS:HA	1.88	0.56
1:B:248:GLN:HE21	1:B:294:LYS:HD2	1.69	0.56
1:A:338:ILE:HD12	1:A:365:VAL:HG21	1.88	0.56
1:A:209:GLU:O	1:A:209:GLU:HG3	2.06	0.56
1:A:245:LYS:HZ2	1:A:251:ASP:HB2	1.71	0.55
1:A:289:ASP:HB3	1:A:291:THR:OG1	2.06	0.55
1:B:315:ARG:HH12	5:B:1010:GOL:H32	1.72	0.54
1:A:188:ARG:HD3	1:A:336:ASP:OD2	2.07	0.54
1:B:391:LEU:C	1:B:391:LEU:HD12	2.27	0.54
1:B:351:LYS:HE2	6:B:1768:HOH:O	2.06	0.54
1:A:532:LEU:HD22	1:A:581:LYS:HG3	1.89	0.54
1:A:254:ASN:HD22	1:A:254:ASN:H	1.55	0.54
1:B:94:ILE:HD12	1:B:109:LYS:HE3	1.90	0.53
1:B:526:ASP:O	1:B:530:GLU:HG3	2.09	0.53
1:A:254:ASN:N	1:A:254:ASN:HD22	2.07	0.53
1:B:536:ARG:NH1	1:B:576:LEU:O	2.41	0.53
1:B:64:ASN:ND2	6:B:1723:HOH:O	2.42	0.53
1:A:532:LEU:HD12	1:A:536:ARG:NE	2.24	0.52
1:B:268:LYS:HG3	6:B:1750:HOH:O	2.09	0.52
1:B:122:LYS:C	1:B:123:MET:HE3	2.30	0.52
1:B:278:GLN:NE2	1:B:299:LYS:HD2	2.24	0.52
1:A:59:VAL:HG13	1:A:60:THR:HG23	1.92	0.52
1:B:533:VAL:HG23	6:B:1283:HOH:O	2.09	0.52
1:A:573:GLU:O	1:A:577:LYS:HD3	2.10	0.52
1:A:237:ILE:HD11	1:A:263:LYS:HD2	1.93	0.51
1:B:315:ARG:HH22	5:B:1010:GOL:H2	1.75	0.51
1:A:532:LEU:HD12	1:A:536:ARG:HE	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:TYR:CZ	1:B:304:LYS:HD3	2.45	0.51
1:B:210:VAL:O	1:B:213:GLU:HG2	2.11	0.51
1:B:285:TYR:N	1:B:295:HIS:HD2	2.08	0.51
1:A:425:VAL:HG11	1:A:428:MET:HE3	1.92	0.50
1:A:4:ILE:HD12	1:A:383:THR:HG23	1.94	0.50
1:A:489:LYS:HE2	6:A:1711:HOH:O	2.12	0.50
1:A:418:ILE:HA	1:A:419:PRO:C	2.32	0.50
1:B:26:VAL:HG23	1:B:373:ILE:HD11	1.94	0.50
1:B:40:ILE:HD13	1:B:115:ILE:HG22	1.94	0.50
1:A:533:VAL:HG23	6:A:1359:HOH:O	2.13	0.49
1:A:427:SER:HB2	1:A:436:VAL:CG2	2.42	0.49
1:B:94:ILE:CD1	1:B:109:LYS:HG2	2.43	0.49
1:B:90:PRO:C	6:B:1737:HOH:O	2.50	0.49
1:A:59:VAL:HA	1:A:260:GLN:HG3	1.95	0.49
1:A:210:VAL:O	1:A:213:GLU:HG2	2.13	0.49
1:B:359:LYS:HE3	6:B:1538:HOH:O	2.12	0.48
1:A:351:LYS:O	1:A:355:GLU:HG3	2.13	0.48
1:B:286:ILE:HG23	1:B:287:THR:HG22	1.96	0.48
1:B:277:GLN:HE21	1:B:277:GLN:HB3	1.54	0.48
1:A:182:ASP:N	1:A:182:ASP:OD1	2.47	0.47
1:B:527:ARG:O	6:B:1573:HOH:O	2.20	0.47
1:B:241:VAL:HG11	1:B:253:ARG:HG3	1.95	0.47
1:A:210:VAL:O	1:A:210:VAL:HG12	2.14	0.47
1:B:210:VAL:O	1:B:210:VAL:HG12	2.13	0.47
1:B:47:GLU:HB2	1:B:529:PHE:CZ	2.50	0.47
1:B:241:VAL:HG11	1:B:253:ARG:CZ	2.45	0.47
1:A:528:LYS:O	1:A:531:GLU:HG3	2.14	0.47
1:B:597:LYS:O	1:B:601:ILE:HG13	2.15	0.47
1:A:425:VAL:HG11	1:A:428:MET:CE	2.46	0.46
1:A:235:ARG:HH21	5:A:1009:GOL:H2	1.80	0.46
1:A:57:GLN:NE2	1:A:61:ASN:HD22	2.11	0.46
1:A:76:ARG:NH1	6:A:1313:HOH:O	2.45	0.46
1:B:532:LEU:HD12	1:B:536:ARG:HE	1.80	0.46
1:B:40:ILE:HD11	1:B:119:VAL:CG2	2.46	0.46
1:A:42:TYR:HA	1:A:47:GLU:O	2.15	0.46
1:A:590:GLU:O	1:A:594:VAL:HG23	2.15	0.46
1:B:261:ARG:NH1	1:B:286:ILE:HA	2.30	0.46
1:A:459:LEU:HD21	1:A:499:ILE:HG12	1.98	0.46
1:B:240:LEU:HD22	1:B:298:ILE:HG21	1.98	0.46
1:B:182:ASP:OD1	1:B:182:ASP:N	2.47	0.46
1:B:527:ARG:HG3	6:B:1620:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TYR:CZ	1:A:304:LYS:HD3	2.50	0.45
1:B:427:SER:HB3	1:B:436:VAL:CG2	2.46	0.45
1:A:52:GLN:N	1:A:53:PRO:CD	2.80	0.45
1:B:64:ASN:ND2	1:B:106:LYS:CE	2.77	0.45
1:B:532:LEU:O	1:B:536:ARG:HG3	2.17	0.45
1:B:248:GLN:NE2	1:B:294:LYS:HD2	2.31	0.45
1:A:59:VAL:HA	1:A:260:GLN:CG	2.47	0.44
1:A:278:GLN:OE1	1:B:536:ARG:CD	2.61	0.44
1:B:174:ALA:O	1:B:374:GLY:HA3	2.18	0.44
1:B:418:ILE:HA	1:B:419:PRO:C	2.38	0.44
1:A:517:ARG:NH2	6:A:1352:HOH:O	2.51	0.43
1:A:235:ARG:HH21	5:A:1009:GOL:C2	2.31	0.43
1:A:112:PRO:HB2	1:A:113:PRO:HD3	2.00	0.43
1:A:532:LEU:CD1	1:A:536:ARG:NE	2.81	0.43
1:A:533:VAL:HG13	1:B:278:GLN:HB2	2.01	0.43
1:A:52:GLN:HB3	1:A:53:PRO:HD3	2.01	0.43
1:B:244:PHE:CE1	1:B:248:GLN:HG3	2.53	0.43
1:B:24:PRO:HB2	1:B:373:ILE:HD12	2.00	0.43
1:B:52:GLN:HB3	1:B:53:PRO:HD3	2.00	0.43
1:A:40:ILE:HD13	1:A:115:ILE:HG22	2.01	0.43
1:A:56:ARG:NH1	1:B:272:GLU:OE1	2.51	0.43
1:B:112:PRO:HB2	1:B:113:PRO:HD3	2.01	0.42
1:A:174:ALA:O	1:A:374:GLY:HA3	2.19	0.42
1:B:528:LYS:C	6:B:1573:HOH:O	2.57	0.42
1:B:52:GLN:HG2	6:B:1761:HOH:O	2.19	0.42
1:A:23:THR:HA	1:A:24:PRO:HD3	1.89	0.42
1:B:102:TRP:CZ2	1:B:111:ALA:HB2	2.55	0.42
1:A:102:TRP:CZ2	1:A:111:ALA:HB2	2.55	0.42
1:A:466:PRO:O	1:A:467:ARG:HB2	2.20	0.42
1:B:90:PRO:HB2	6:B:1737:HOH:O	2.20	0.41
1:A:124:LYS:HE2	1:A:135:VAL:O	2.20	0.41
1:A:391:LEU:HD12	1:A:391:LEU:C	2.39	0.41
1:B:62:PRO:C	6:B:1737:HOH:O	2.58	0.41
1:B:403:THR:OG1	1:B:407:VAL:HG23	2.20	0.41
1:B:532:LEU:HD12	1:B:536:ARG:NE	2.36	0.41
1:B:338:ILE:HD12	1:B:365:VAL:HG21	2.02	0.41
1:A:58:ALA:HB1	6:A:1554:HOH:O	2.21	0.41
1:A:289:ASP:OD1	1:A:290:ALA:N	2.54	0.41
1:A:306:GLU:HB3	1:A:348:MET:CE	2.50	0.41
1:B:254:ASN:C	1:B:254:ASN:ND2	2.74	0.41
1:B:94:ILE:HD11	1:B:109:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:OE2	1:B:56:ARG:NH1	2.49	0.40
1:B:269:ALA:HB1	1:B:279:THR:HG21	2.03	0.40
1:A:532:LEU:CD2	1:A:581:LYS:HB2	2.51	0.40
1:B:52:GLN:N	1:B:53:PRO:CD	2.84	0.40
1:A:532:LEU:O	1:A:536:ARG:HG3	2.22	0.40
1:B:229:GLY:HA3	3:B:1002:ATP:O3'	2.22	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	598/608 (98%)	592 (99%)	6 (1%)	0	100	100
1	B	598/608 (98%)	593 (99%)	5 (1%)	0	100	100
All	All	1196/1216 (98%)	1185 (99%)	11 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	489/495 (99%)	478 (98%)	11 (2%)	60	51
1	B	489/495 (99%)	474 (97%)	15 (3%)	47	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	978/990 (99%)	952 (97%)	26 (3%)	52	41

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	57	GLN
1	A	146	PHE
1	A	182	ASP
1	A	210	VAL
1	A	247	ASP
1	A	254	ASN
1	A	332	SER
1	A	456	GLN
1	A	529	PHE
1	A	532	LEU
1	B	22	THR
1	B	57	GLN
1	B	123	MET
1	B	125	LYS
1	B	146	PHE
1	B	182	ASP
1	B	210	VAL
1	B	254	ASN
1	B	277	GLN
1	B	304	LYS
1	B	427	SER
1	B	437	THR
1	B	456	GLN
1	B	532	LEU
1	B	570	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	57	GLN
1	A	254	ASN
1	A	277	GLN
1	A	295	HIS
1	A	458	ASN

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Mol	Chain	Res	Type
1	A	544	HIS
1	B	57	GLN
1	B	64	ASN
1	B	248	GLN
1	B	254	ASN
1	B	277	GLN
1	B	295	HIS
1	B	458	ASN
1	B	589	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
3	ATP	A	1002	2	24,33,33	0.98	1 (4%)	31,52,52	1.81	4 (12%)
4	SO4	A	1003	-	4,4,4	0.25	0	6,6,6	0.07	0
4	SO4	A	1004	-	4,4,4	0.23	0	6,6,6	0.10	0
4	SO4	A	1005	-	4,4,4	0.22	0	6,6,6	0.10	0
4	SO4	A	1006	-	4,4,4	0.15	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	1007	-	4,4,4	0.21	0	6,6,6	0.06	0
5	GOL	A	1008	-	5,5,5	0.36	0	5,5,5	0.42	0
5	GOL	A	1009	-	5,5,5	0.37	0	5,5,5	0.18	0
3	ATP	B	1002	2	24,33,33	0.93	1 (4%)	31,52,52	1.80	4 (12%)
4	SO4	B	1003	-	4,4,4	0.19	0	6,6,6	0.12	0
4	SO4	B	1004	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	B	1005	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	B	1006	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	B	1007	-	4,4,4	0.19	0	6,6,6	0.07	0
4	SO4	B	1008[A]	-	4,4,4	0.28	0	6,6,6	0.09	0
4	SO4	B	1008[B]	-	4,4,4	0.24	0	6,6,6	0.08	0
5	GOL	B	1009	-	5,5,5	0.31	0	5,5,5	0.25	0
5	GOL	B	1010	-	5,5,5	0.34	0	5,5,5	0.21	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	ATP	A	1002	2	-	0/18/38/38	0/3/3/3
4	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1008	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1009	-	-	0/4/4/4	0/0/0/0
3	ATP	B	1002	2	-	0/18/38/38	0/3/3/3
4	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1004	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1007	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1008[A]	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1008[B]	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1009	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1010	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	ATP	C5-C4	2.78	1.46	1.40
3	A	1002	ATP	C5-C4	2.95	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	ATP	N3-C2-N1	-7.37	123.25	128.89
3	A	1002	ATP	N3-C2-N1	-7.24	123.35	128.89
3	B	1002	ATP	C1'-N9-C4	-2.93	122.53	126.94
3	A	1002	ATP	C1'-N9-C4	-2.85	122.63	126.94
3	B	1002	ATP	C4-C5-N7	-2.79	106.92	109.48
3	A	1002	ATP	C4-C5-N7	-2.56	107.13	109.48
3	A	1002	ATP	PA-O3A-PB	-2.23	126.45	132.73
3	B	1002	ATP	PA-O3A-PB	-2.01	127.07	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1008	GOL	1	0
5	A	1009	GOL	2	0
3	B	1002	ATP	1	0
5	B	1010	GOL	2	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	600/608 (98%)	0.33	43 (7%) 18 28	13, 26, 60, 112	0
1	B	600/608 (98%)	0.38	46 (7%) 16 25	11, 26, 69, 119	0
All	All	1200/1216 (98%)	0.35	89 (7%) 17 27	11, 26, 62, 119	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	VAL	13.3
1	A	210	VAL	9.6
1	B	601	ILE	9.3
1	B	211	ASP	7.4
1	B	555	ASP	6.8
1	B	604	GLN	6.5
1	B	559	ALA	6.4
1	B	560	ASP	6.4
1	A	211	ASP	6.3
1	B	183	LYS	6.3
1	B	556	LYS	6.0
1	B	563	THR	6.0
1	B	557	LEU	5.8
1	A	601	ILE	5.7
1	A	212	GLY	5.5
1	A	555	ASP	5.5
1	A	183	LYS	5.3
1	B	598	LEU	4.8
1	B	565	ILE	4.7
1	B	558	PRO	4.6
1	B	564	ALA	4.4
1	A	554	GLY	4.1
1	A	557	LEU	4.1
1	B	209	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	GLY	4.1
1	A	209	GLU	4.0
1	B	561	ASP	3.9
1	B	554	GLY	3.8
1	B	597	LYS	3.7
1	A	185	THR	3.7
1	A	290	ALA	3.7
1	A	556	LYS	3.5
1	A	564	ALA	3.5
1	B	527	ARG	3.4
1	B	186	GLY	3.4
1	B	553	ALA	3.4
1	A	604	GLN	3.3
1	A	42	TYR	3.3
1	A	532	LEU	3.3
1	B	532	LEU	3.3
1	B	562	LYS	3.3
1	A	390	LEU	3.3
1	A	1	SER	3.3
1	B	551	GLU	3.2
1	A	559	ALA	3.1
1	B	254	ASN	3.1
1	A	565	ILE	3.0
1	A	553	ALA	3.0
1	A	529	PHE	3.0
1	A	184	GLY	3.0
1	A	186	GLY	3.0
1	A	288	ALA	2.9
1	A	292	GLY	2.9
1	A	527	ARG	2.9
1	B	108	GLN	2.8
1	B	533	VAL	2.8
1	B	253	ARG	2.6
1	A	45	ASP	2.6
1	B	46	GLY	2.6
1	A	598	LEU	2.5
1	B	185	THR	2.5
1	A	291	THR	2.5
1	A	289	ASP	2.5
1	B	184	GLY	2.5
1	A	9	LEU	2.5
1	B	288	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	529	PHE	2.4
1	B	600	GLU	2.4
1	B	567	SER	2.4
1	A	558	PRO	2.3
1	A	563	THR	2.2
1	A	550	VAL	2.2
1	B	384	GLY	2.2
1	B	514	LYS	2.2
1	A	208	ASP	2.2
1	A	43	THR	2.2
1	A	560	ASP	2.1
1	B	256	PRO	2.1
1	B	1	SER	2.1
1	B	390	LEU	2.1
1	B	286	ILE	2.1
1	B	213	GLU	2.1
1	A	602	ALA	2.1
1	A	254	ASN	2.1
1	A	597	LYS	2.0
1	B	603	GLN	2.1
1	A	87	SER	2.0
1	B	107	GLY	2.0
1	A	108	GLN	2.0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	SO4	B	1006	5/5	0.94	0.18	6.21	31,43,69,74	0
4	SO4	A	1006	5/5	0.94	0.17	4.80	29,41,70,76	0
4	SO4	B	1007	5/5	0.97	0.27	4.19	53,54,59,67	0
5	GOL	A	1009	6/6	0.86	0.23	3.72	68,82,92,94	0
5	GOL	A	1008	6/6	0.89	0.17	3.41	27,46,56,56	0
5	GOL	B	1010	6/6	0.93	0.15	3.37	42,60,72,82	0
4	SO4	A	1007	5/5	0.98	0.22	2.41	41,44,45,53	0
2	MG	B	1001	1/1	0.99	0.18	0.61	18,18,18,18	0
2	MG	A	1001	1/1	0.99	0.17	0.13	18,18,18,18	0
3	ATP	B	1002	31/31	0.99	0.12	-0.40	10,14,19,21	0
4	SO4	A	1003	5/5	0.99	0.10	-0.60	38,42,48,50	0
3	ATP	A	1002	31/31	0.99	0.11	-0.60	11,16,21,22	0
5	GOL	B	1009	6/6	0.97	0.07	-1.42	22,31,39,39	0
4	SO4	B	1008[A]	5/5	0.94	0.15	-	29,41,42,52	5
4	SO4	A	1004	5/5	0.94	0.23	-	60,74,78,88	0
4	SO4	B	1005	5/5	0.92	0.22	-	71,79,79,85	0
4	SO4	B	1003	5/5	0.98	0.09	-	37,38,39,47	0
4	SO4	B	1004	5/5	0.97	0.12	-	70,72,74,80	0
4	SO4	B	1008[B]	5/5	0.94	0.15	-	39,41,43,44	5
4	SO4	A	1005	5/5	0.91	0.19	-	73,75,77,84	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.