



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2017 – 08:56 pm GMT

PDB ID : 5MB9  
Title : Crystal structure of the eukaryotic ribosome associated complex (RAC), a unique Hsp70/Hsp40 pair  
Authors : Gumiero, A.; Weyer, F.A.; Valentin Gese, G.; Lapouge, K.; Sinning, I.  
Deposited on : 2016-11-07  
Resolution : 3.20 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : recalc29047  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc29047

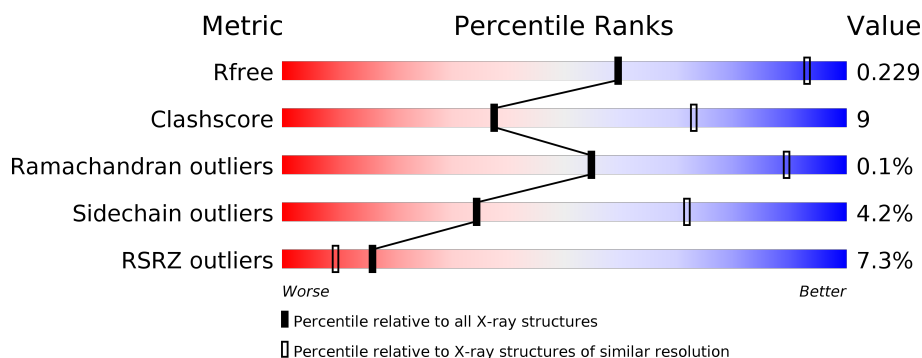
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	590	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	590	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>17%</div> </div> </div>
2	C	45	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>11%</div> <div></div> <div>36%</div> </div> </div>
2	D	45	<div> <div>16%</div> <div> <div></div> <div>69%</div> <div>9%</div> <div></div> <div>22%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8185 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 Putative heat shock protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3845	2412	672	758	3			
1	B	491	Total	C	N	O	S	0	0	0
			3750	2354	651	742	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	SER	-	expression tag	UNP G0RZX9
A	-10	ALA	-	expression tag	UNP G0RZX9
A	-9	MET	-	expression tag	UNP G0RZX9
A	-8	GLY	-	expression tag	UNP G0RZX9
A	-7	TRP	-	expression tag	UNP G0RZX9
A	-6	SER	-	expression tag	UNP G0RZX9
A	-5	HIS	-	expression tag	UNP G0RZX9
A	-4	PRO	-	expression tag	UNP G0RZX9
A	-3	GLN	-	expression tag	UNP G0RZX9
A	-2	PHE	-	expression tag	UNP G0RZX9
A	-1	GLU	-	expression tag	UNP G0RZX9
A	0	LYS	-	expression tag	UNP G0RZX9
B	-11	SER	-	expression tag	UNP G0RZX9
B	-10	ALA	-	expression tag	UNP G0RZX9
B	-9	MET	-	expression tag	UNP G0RZX9
B	-8	GLY	-	expression tag	UNP G0RZX9
B	-7	TRP	-	expression tag	UNP G0RZX9
B	-6	SER	-	expression tag	UNP G0RZX9
B	-5	HIS	-	expression tag	UNP G0RZX9
B	-4	PRO	-	expression tag	UNP G0RZX9
B	-3	GLN	-	expression tag	UNP G0RZX9
B	-2	PHE	-	expression tag	UNP G0RZX9
B	-1	GLU	-	expression tag	UNP G0RZX9
B	0	LYS	-	expression tag	UNP G0RZX9

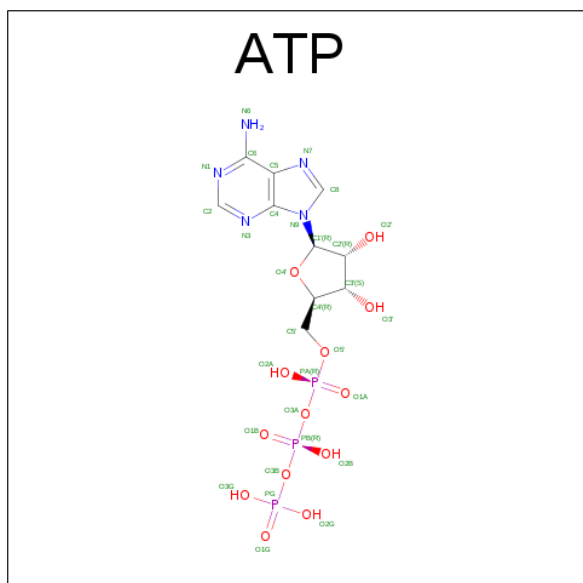
- Molecule 2 is a protein called Putative ribosome associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	29	Total	C	N	O	S	0	0	0
			236	145	52	38	1			
2	D	35	Total	C	N	O	S	0	0	0
			276	174	57	44	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLY	-	expression tag	UNP G0RYD6
C	17	ALA	-	expression tag	UNP G0RYD6
C	18	MET	-	expression tag	UNP G0RYD6
D	16	GLY	-	expression tag	UNP G0RYD6
D	17	ALA	-	expression tag	UNP G0RYD6
D	18	MET	-	expression tag	UNP G0RYD6

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



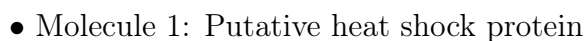
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0

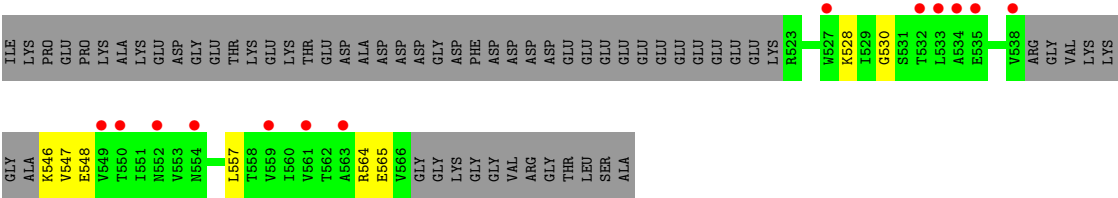
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0
6	B	4	Total O 4 4	0	0



- Molecule 1: Putative heat shock protein

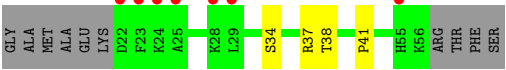




● Molecule 2: Putative ribosome associated protein



● Molecule 2: Putative ribosome associated protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.92Å 179.36Å 155.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 3.20 47.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.97-3.20) 99.4 (47.97-3.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.227 , 0.285 0.221 , 0.229	Depositor DCC
$R_{free}$ test set	1096 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	96.9	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8185	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: GOL, MG, 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	0.26	0/3903	0.47	0/5301
1	B	0.25	0/3807	0.47	0/5176
2	C	0.25	0/241	0.41	0/322
2	D	0.27	0/282	0.42	0/376
All	All	0.26	0/8233	0.47	0/11175

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 [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	3845	0	3876	74	0
1	B	3750	0	3766	70	0
2	C	236	0	241	5	0
2	D	276	0	284	5	0
3	A	31	0	12	2	0
3	B	31	0	12	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	4	0	0	1	0
6	B	4	0	0	1	0
All	All	8185	0	8199	144	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 (144) 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:20:PHE:O	1:A:80:ARG:NH1	2.03	0.90
1:A:225:ARG:NH1	1:A:446:PRO:O	2.10	0.85
1:B:428:GLY:HA2	1:B:443:ILE:HG22	1.59	0.84
1:B:40:ASN:ND2	1:B:60:TYR:OH	2.11	0.83
1:A:29:HIS:HB3	1:A:38:ILE:HD11	1.73	0.70
1:A:426:ALA:HB2	1:A:446:PRO:HD3	1.75	0.69
1:B:58:GLU:O	1:B:137:ARG:NH2	2.26	0.69
1:B:230:THR:HG21	1:B:422:HIS:HE1	1.59	0.68
1:A:31:VAL:HG12	1:A:34:LYS:H	1.58	0.68
1:B:351:SER:HB3	1:B:389:LEU:HD12	1.77	0.67
1:A:548:GLU:O	1:A:565:GLU:HB3	1.94	0.67
1:B:426:ALA:HB2	1:B:446:PRO:HD3	1.78	0.64
1:A:469:VAL:HG23	1:A:536:ALA:HB3	1.79	0.64
1:B:13:ARG:NH1	1:B:179:GLU:OE1	2.30	0.64
1:A:27:ILE:HD12	1:A:142:ALA:HB2	1.79	0.64
1:B:230:THR:HG22	2:C:39:LEU:HG	1.82	0.62
1:B:365:ARG:NH2	1:B:372:THR:O	2.32	0.61
1:B:413:THR:O	1:B:417:VAL:HB	2.01	0.61
1:A:16:ILE:HD12	1:A:150:VAL:HG11	1.82	0.61
1:A:430:VAL:HG11	1:A:470:LYS:HE2	1.83	0.60
1:A:191:VAL:HG22	1:A:349:ILE:HD12	1.84	0.59
1:A:18:ILE:HG12	1:A:27:ILE:HG22	1.84	0.59
1:A:223:ALA:HB3	1:A:230:THR:HG23	1.85	0.59
1:B:418:THR:HA	2:C:38:THR:HG22	1.84	0.59
1:B:197:ARG:NH2	1:B:199:GLU:OE2	2.36	0.58
1:A:547:VAL:HG13	1:A:565:GLU:HG3	1.86	0.58
3:B:601:ATP:O2G	6:B:701:HOH:O	2.17	0.58
1:A:347:GLU:HG2	1:A:373:ARG:HB3	1.86	0.58
1:A:80:ARG:NH2	6:A:803:HOH:O	2.36	0.57
1:A:466:ASP:HB3	1:A:539:ARG:HA	1.88	0.56
1:A:224:SER:C	1:A:225:ARG:HD2	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:SD	2:C:49:HIS:NE2	2.78	0.56
1:A:15:VAL:HG11	1:A:402:GLN:HB3	1.88	0.55
1:A:80:ARG:NH2	1:A:186:GLU:OE2	2.35	0.55
1:B:286:ARG:HG2	3:B:601:ATP:C5	2.42	0.55
1:A:466:ASP:N	1:A:466:ASP:OD1	2.17	0.54
1:A:337:LYS:HG3	1:B:262:PRO:HB3	1.89	0.54
1:A:422:HIS:CD2	2:D:37:ARG:HB2	2.43	0.54
1:B:196:ALA:HB3	1:B:396:LEU:HD13	1.90	0.54
1:B:266:ASP:OD2	1:B:268:ARG:NH2	2.31	0.53
1:B:82:ILE:HD12	1:B:90:VAL:HG13	1.90	0.53
1:A:447:GLU:OE1	2:D:37:ARG:NH1	2.42	0.53
1:B:208:VAL:HG22	1:B:221:VAL:HG12	1.89	0.53
1:A:422:HIS:CE1	1:A:449:ALA:HB2	2.44	0.53
1:B:444:ILE:HG12	1:B:454:ARG:HG3	1.90	0.52
1:A:254:SER:OG	1:A:268:ARG:HD2	2.10	0.52
1:A:237:ASP:HB2	1:A:330:LEU:HD21	1.93	0.51
1:B:13:ARG:HB3	1:B:151:THR:OG1	2.09	0.51
1:B:368:PHE:HB3	1:B:372:THR:HG21	1.93	0.51
1:A:82:ILE:HG23	1:A:90:VAL:HG11	1.92	0.51
1:B:112:ILE:HD11	1:B:125:LEU:HD12	1.92	0.51
1:B:109:VAL:HG12	1:B:126:THR:HA	1.92	0.51
1:A:212:LEU:HB3	1:A:354:THR:HB	1.93	0.51
1:B:22:ASN:HD21	1:B:81:ASP:H	1.59	0.51
1:A:157:ILE:HD12	1:A:161:PHE:HE2	1.76	0.50
1:A:191:VAL:HG21	1:A:222:LEU:HD12	1.93	0.50
1:B:84:GLY:HA3	1:B:165:GLN:HA	1.92	0.50
1:B:129:GLU:O	1:B:133:ARG:HG3	2.12	0.50
1:B:221:VAL:HG21	1:B:338:ALA:HB2	1.94	0.50
1:B:82:ILE:HB	1:B:127:VAL:HG21	1.94	0.50
1:A:445:ALA:O	1:A:448:THR:OG1	2.23	0.49
1:B:557:LEU:HB3	2:C:29:LEU:HD12	1.94	0.49
1:B:221:VAL:HG22	1:B:233:ALA:HB3	1.94	0.49
1:A:83:LEU:O	1:A:165:GLN:HG2	2.13	0.49
1:B:422:HIS:CE1	1:B:449:ALA:HB2	2.47	0.49
1:A:455:THR:HB	1:A:550:THR:HB	1.94	0.49
1:A:208:VAL:HG22	1:A:221:VAL:HG22	1.95	0.48
1:A:52:SER:HB2	1:A:75:THR:HG23	1.95	0.48
1:B:204:ASP:OD1	1:B:204:ASP:N	2.46	0.48
1:A:397:GLN:NE2	1:A:401:ILE:HD11	2.29	0.47
1:A:206:ILE:HD13	1:A:340:LEU:HD21	1.95	0.47
1:B:83:LEU:O	1:B:165:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:O	1:A:90:VAL:HG22	2.14	0.47
1:B:473:GLU:HB2	1:B:530:GLY:HA3	1.97	0.47
1:A:204:ASP:HA	1:A:224:SER:O	2.14	0.47
1:A:197:ARG:NH2	1:A:382:SER:O	2.42	0.47
1:A:109:VAL:HG12	1:A:126:THR:HA	1.97	0.46
1:B:467:VAL:HG21	1:B:547:VAL:HG11	1.97	0.46
1:A:18:ILE:HB	1:A:155:ILE:HD13	1.98	0.46
1:A:83:LEU:HD23	1:A:127:VAL:HG22	1.98	0.45
1:B:258:LEU:HD21	1:B:266:ASP:HA	1.98	0.45
1:B:546:LYS:O	1:B:565:GLU:HG3	2.16	0.45
1:B:351:SER:HA	1:B:386:PRO:HB3	1.99	0.45
1:B:162:THR:O	1:B:166:LYS:HG3	2.17	0.45
1:B:317:GLU:CD	1:B:359:ARG:HG3	2.37	0.45
1:B:405:GLU:HG3	1:B:407:GLU:H	1.81	0.45
1:A:49:THR:HA	1:A:134:TYR:CZ	2.52	0.45
1:A:157:ILE:HB	1:A:161:PHE:CZ	2.52	0.45
1:A:16:ILE:HD11	1:A:150:VAL:HG21	1.98	0.45
1:A:157:ILE:HG12	1:A:184:ILE:O	2.16	0.45
1:A:418:THR:HA	2:D:38:THR:HG23	1.98	0.45
1:A:430:VAL:HG12	1:A:470:LYS:HB3	1.98	0.44
1:A:289:SER:OG	3:A:700:ATP:N1	2.47	0.44
1:A:456:VAL:O	1:A:548:GLU:HA	2.18	0.44
1:B:241:HIS:CE1	1:B:243:ILE:HB	2.53	0.44
1:A:225:ARG:HD2	1:A:225:ARG:N	2.33	0.44
1:A:413:THR:O	1:A:417:VAL:HB	2.17	0.44
1:A:106:ASP:N	1:A:106:ASP:OD1	2.49	0.43
1:B:411:GLN:HA	1:B:414:HIS:CE1	2.53	0.43
1:A:421:PRO:HB2	2:D:34:SER:OG	2.18	0.43
1:A:208:VAL:HG22	1:A:221:VAL:HG13	2.00	0.43
1:A:415:ALA:O	1:A:419:THR:OG1	2.30	0.43
1:B:20:PHE:CD2	1:B:80:ARG:HG2	2.53	0.43
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.85	0.43
1:A:365:ARG:NH2	1:A:372:THR:O	2.52	0.43
1:A:470:LYS:HG3	1:A:535:GLU:HG3	2.01	0.43
1:B:528:LYS:HA	1:B:528:LYS:HD3	1.88	0.42
1:A:225:ARG:HG2	1:A:448:THR:HA	2.02	0.42
1:A:29:HIS:CE1	1:A:36:GLU:HB2	2.54	0.42
1:B:250:ILE:HD11	1:B:278:ARG:HA	2.01	0.42
1:B:289:SER:OG	3:B:601:ATP:N1	2.37	0.42
1:B:422:HIS:CD2	2:C:37:ARG:HB2	2.54	0.42
1:A:136:ARG:NH2	1:A:175:ALA:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASN:HD21	1:A:74:ASN:HB2	1.84	0.42
1:B:18:ILE:HG12	1:B:27:ILE:HG22	2.01	0.42
1:B:285:LYS:HE3	3:B:601:ATP:N3	2.35	0.42
1:A:427:ILE:HD11	1:A:444:ILE:HD12	2.00	0.42
1:B:208:VAL:HB	1:B:348:VAL:HG12	2.00	0.42
1:B:237:ASP:HB2	1:B:330:LEU:HD21	2.01	0.42
1:B:14:VAL:HG23	1:B:150:VAL:HA	2.01	0.42
1:A:464:GLY:HA2	1:A:543:LYS:HD3	2.02	0.42
1:B:102:GLN:HE21	1:B:102:GLN:HB3	1.72	0.42
1:B:170:ILE:HA	1:B:180:VAL:HG21	2.02	0.42
1:B:401:ILE:HG23	1:B:409:ILE:HG21	2.01	0.42
1:B:397:GLN:HA	1:B:400:LEU:HD13	2.01	0.41
1:B:282:GLU:HG3	3:B:601:ATP:O2'	2.21	0.41
1:B:403:GLU:HG2	1:B:403:GLU:H	1.66	0.41
1:B:421:PRO:HD2	1:B:450:VAL:HG22	2.02	0.41
1:B:230:THR:HG21	1:B:422:HIS:CE1	2.47	0.41
1:A:82:ILE:HB	1:A:127:VAL:HG21	2.03	0.41
1:A:548:GLU:H	1:A:565:GLU:HB2	1.86	0.41
1:B:26:SER:OG	1:B:391:ALA:HB2	2.20	0.41
1:B:396:LEU:O	1:B:400:LEU:HD12	2.21	0.41
1:A:182:GLN:HE22	2:D:41:PRO:HG2	1.86	0.41
1:A:363:ASN:O	1:A:367:ILE:HG12	2.21	0.41
1:A:24:ASN:HB2	3:A:700:ATP:O1A	2.21	0.41
1:B:427:ILE:HG13	1:B:444:ILE:HB	2.03	0.40
1:B:474:GLY:HA2	1:B:528:LYS:O	2.21	0.40
1:A:427:ILE:HD13	1:A:551:ILE:HD13	2.03	0.40
1:B:225:ARG:HD3	1:B:225:ARG:HH11	1.77	0.40
1:B:60:TYR:CD2	1:B:137:ARG:HG2	2.56	0.40
1:B:456:VAL:O	1:B:548:GLU:HA	2.20	0.40
1:A:466:ASP:HB3	1:A:539:ARG:O	2.22	0.40
1:B:353:GLY:O	1:B:356:ASN:ND2	2.54	0.40

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	497/590 (84%)	480 (97%)	17 (3%)	0	100	100
1	B	481/590 (82%)	468 (97%)	12 (2%)	1 (0%)	51	86
2	C	27/45 (60%)	26 (96%)	1 (4%)	0	100	100
2	D	33/45 (73%)	33 (100%)	0	0	100	100
All	All	1038/1270 (82%)	1007 (97%)	30 (3%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	468	LEU

### 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	417/484 (86%)	398 (95%)	19 (5%)	31	70
1	B	409/484 (84%)	391 (96%)	18 (4%)	33	70
2	C	25/36 (69%)	25 (100%)	0	100	100
2	D	28/36 (78%)	28 (100%)	0	100	100
All	All	879/1040 (84%)	842 (96%)	37 (4%)	34	72

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	31	VAL
1	A	80	ARG
1	A	161	PHE
1	A	216	ARG
1	A	225	ARG
1	A	230	THR

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Mol	Chain	Res	Type
1	A	268	ARG
1	A	359	ARG
1	A	365	ARG
1	A	412	SER
1	A	417	VAL
1	A	441	VAL
1	A	466	ASP
1	A	481	ILE
1	A	522	LYS
1	A	525	LYS
1	A	550	THR
1	A	564	ARG
1	B	34	LYS
1	B	60	TYR
1	B	102	GLN
1	B	137	ARG
1	B	161	PHE
1	B	229	TYR
1	B	315	ARG
1	B	321	ARG
1	B	346	ASP
1	B	359	ARG
1	B	365	ARG
1	B	409	ILE
1	B	412	SER
1	B	414	HIS
1	B	441	VAL
1	B	456	VAL
1	B	457	HIS
1	B	564	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	HIS
1	B	40	ASN
1	B	422	HIS

### 5.3.3 RNA ⓘ

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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	700	4	27,33,33	0.88	1 (3%)	25,52,52	1.64	2 (8%)
3	ATP	B	601	4	27,33,33	0.94	1 (3%)	25,52,52	1.61	2 (8%)
5	GOL	B	603	-	5,5,5	0.36	0	5,5,5	0.18	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	700	4	-	0/18/38/38	0/3/3/3
3	ATP	B	601	4	-	0/18/38/38	0/3/3/3
5	GOL	B	603	-	-	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	A	700	ATP	C5-C4	2.91	1.47	1.40
3	B	601	ATP	C5-C4	3.09	1.47	1.40

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	ATP	N3-C2-N1	-6.00	123.63	128.86
3	A	700	ATP	N3-C2-N1	-5.93	123.70	128.86
3	B	601	ATP	C4-C5-N7	-2.96	106.55	109.41
3	A	700	ATP	C4-C5-N7	-2.87	106.63	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	700	ATP	2	0
3	B	601	ATP	5	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	505/590 (85%)	0.37	32 (6%) 21 12	56, 102, 168, 223	0
1	B	491/590 (83%)	0.44	37 (7%) 15 8	49, 96, 182, 287	0
2	C	29/45 (64%)	0.29	1 (3%) 46 30	85, 127, 171, 235	0
2	D	35/45 (77%)	0.85	7 (20%) 1 1	98, 156, 196, 248	0
All	All	1060/1270 (83%)	0.41	77 (7%) 16 9	49, 102, 177, 287	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	VAL	6.1
1	B	470	LYS	5.9
1	A	537	ALA	5.2
1	B	534	ALA	5.1
1	B	455	THR	4.8
1	B	429	VAL	4.6
1	B	535	GLU	4.5
1	B	428	GLY	4.5
1	B	452	ALA	4.5
1	B	549	VAL	4.4
2	D	29	LEU	4.2
1	B	538	VAL	4.1
1	B	532	THR	4.0
1	B	561	VAL	4.0
1	A	535	GLU	4.0
1	A	15	VAL	4.0
1	A	470	LYS	3.9
2	D	24	LYS	3.9
1	A	549	VAL	3.8
1	B	559	VAL	3.8
1	A	124	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	28	LYS	3.7
1	A	536	ALA	3.7
1	A	469	VAL	3.6
2	D	22	ASP	3.6
1	B	430	VAL	3.5
1	B	444	ILE	3.4
1	A	457	HIS	3.2
1	A	561	VAL	3.1
1	B	550	THR	3.1
1	A	564	ARG	3.1
1	B	265	LYS	3.0
1	A	467	VAL	3.0
1	A	563	ALA	3.0
1	A	565	GLU	3.0
1	B	469	VAL	3.0
1	B	456	VAL	3.0
1	B	229	TYR	3.0
1	B	119	ASP	2.9
1	B	471	VAL	2.8
1	A	207	ILE	2.8
1	A	178	LEU	2.8
1	A	263	GLY	2.8
1	A	125	LEU	2.8
1	B	533	LEU	2.8
1	B	296	PHE	2.8
1	A	429	VAL	2.7
1	B	554	ASN	2.7
1	A	439	LYS	2.7
2	D	23	PHE	2.7
1	B	468	LEU	2.7
1	B	419	THR	2.7
1	A	559	VAL	2.7
1	A	16	ILE	2.6
2	D	25	ALA	2.6
1	A	110	PHE	2.6
2	D	55	HIS	2.5
1	A	552	ASN	2.5
1	A	551	ILE	2.5
1	B	563	ALA	2.5
1	A	468	LEU	2.4
1	B	527	TRP	2.4
1	A	471	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	426	ALA	2.4
1	B	316	TYR	2.3
1	B	552	ASN	2.3
1	B	480	VAL	2.3
1	B	277	LEU	2.3
1	A	560	ILE	2.3
1	B	443	ILE	2.2
2	C	29	LEU	2.2
1	A	188	ALA	2.2
1	B	457	HIS	2.1
1	A	150	VAL	2.1
1	A	534	ALA	2.1
1	A	443	ILE	2.1
1	B	445	ALA	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(Å <sup>2</sup> )	Q<0.9
3	ATP	B	601	31/31	0.95	0.22	-0.06	53,72,96,105	0
3	ATP	A	700	31/31	0.96	0.22	-0.31	56,66,80,94	0
4	MG	B	602	1/1	0.96	0.15	-	67,67,67,67	0
4	MG	A	701	1/1	0.98	0.24	-	70,70,70,70	0
5	GOL	B	603	6/6	0.58	0.25	-	97,103,112,113	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.