



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 PM GMT

PDB ID : 4J0B  
Title : Structure of mitochondrial Hsp90 (TRAP1) with ADP-BeF3  
Authors : Partridge, J.R.; Lavery, L.A.; Agard, D.A.  
Deposited on : 2013-01-30  
Resolution : 2.35 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

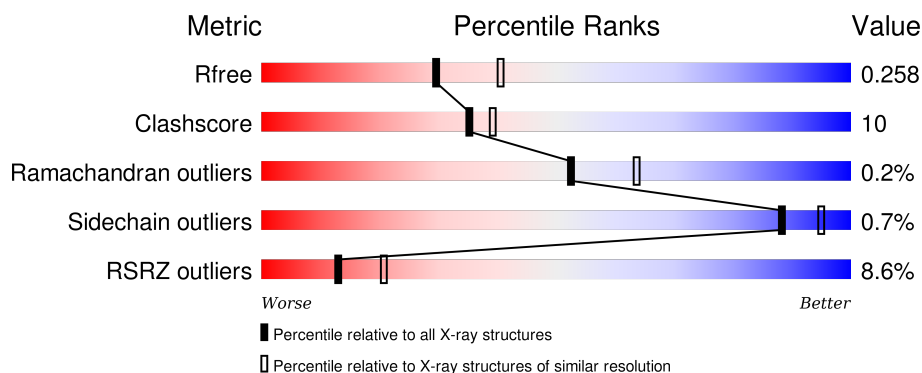
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	647	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>8%</div> </div> </div>
1	B	647	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9953 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 TNF receptor-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	594	Total	C	N	O	S	0	0	0
			4764	3017	826	900	21			
1	B	609	Total	C	N	O	S	0	4	0
			4934	3130	853	927	24			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

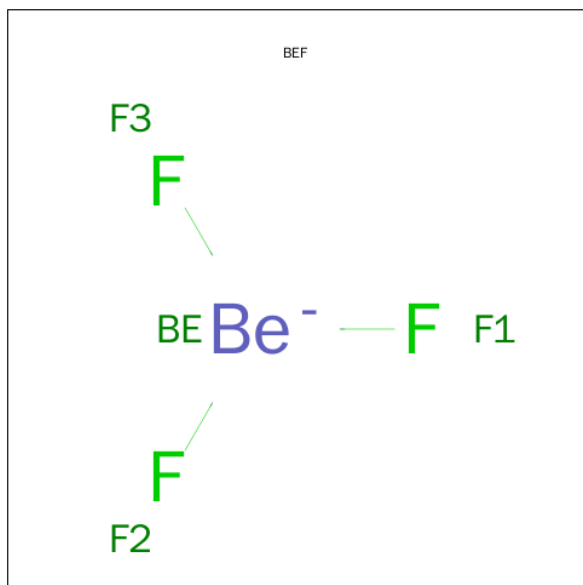
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Co	0	0
			2	2		
2	A	2	Total	Co	0	0
			2	2		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	90	Total	O	0	0
			90	90		

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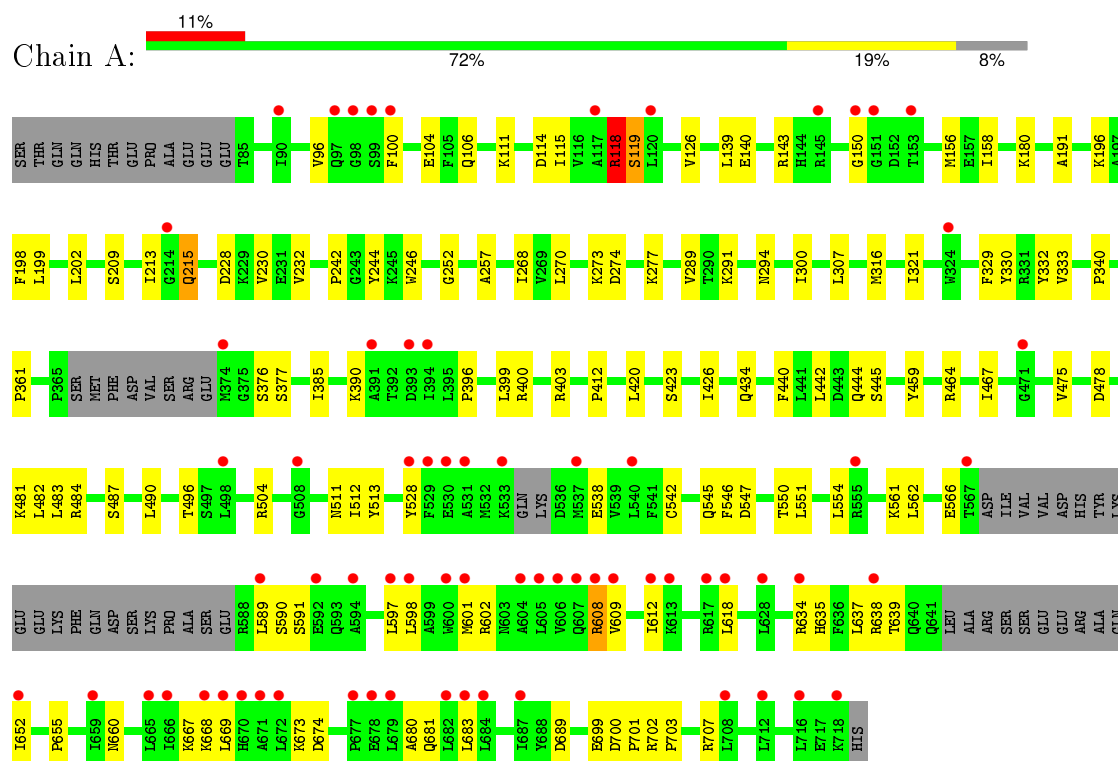
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	97	Total	O	0	0
			97	97		

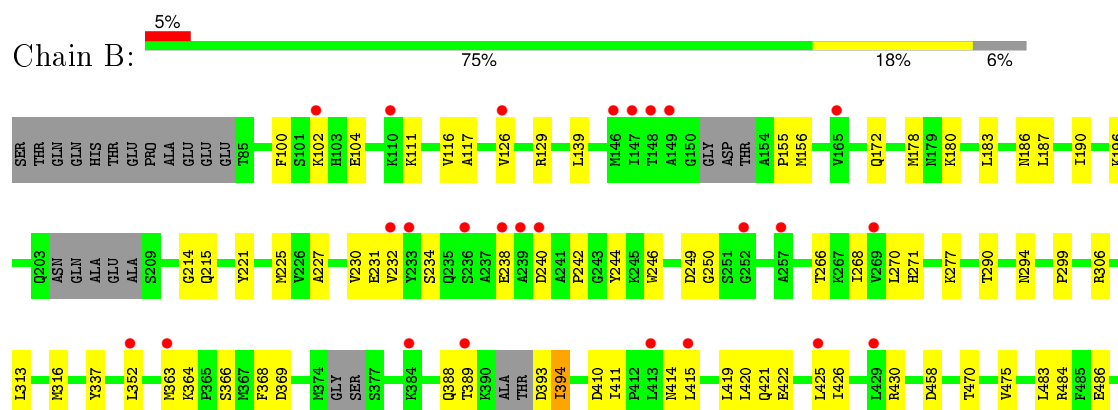
### 3 Residue-property plots

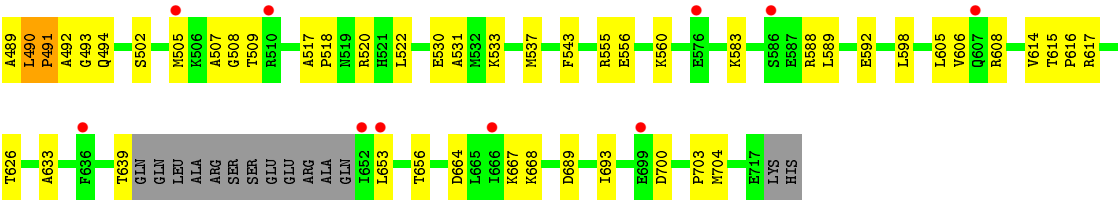
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: TNF receptor-associated protein 1



#### • Molecule 1: TNF receptor-associated protein 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.78 Å   96.57 Å   124.98 Å 90.00°   134.29°   90.00°	Depositor
Resolution (Å)	29.82 – 2.35 42.49 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.82-2.35) 90.9 (42.49-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.34 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1278)	Depositor
R, $R_{free}$	0.205   ,   0.248 0.221   ,   0.258	Depositor DCC
$R_{free}$ test set	2030 reflections (3.67%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 52.3	EDS
Estimated twinning fraction	0.000 for h+2*l,k,-h-l 0.008 for h,-k,-h-l 0.010 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 62277 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: CO, MG, BEF, ADP

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	0.42	0/4849	0.61	2/6536 (0.0%)
1	B	0.41	1/5035 (0.0%)	0.61	4/6780 (0.1%)
All	All	0.42	1/9884 (0.0%)	0.61	6/13316 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	491	PRO	N-CD	5.10	1.54	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	GLY	N-CA-C	5.99	128.08	113.10
1	B	639	THR	N-CA-CB	5.95	121.61	110.30
1	B	215	GLN	N-CA-CB	-5.71	100.31	110.60
1	B	490	LEU	C-N-CD	5.70	140.38	128.40
1	A	118	ARG	N-CA-CB	-5.30	101.05	110.60
1	A	608	ARG	N-CA-C	5.02	124.56	111.00

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	4764	0	4770	104	0
1	B	4934	0	4950	99	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	90	0	0	1	0
6	B	97	0	0	0	0
All	All	9953	0	9744	191	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 10.

All (191) 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:414:ASN:ND2	1:B:419:LEU:HB2	1.43	1.30
1:A:490:LEU:CD1	1:A:496:THR:CG2	2.31	1.09
1:A:490:LEU:CD1	1:A:496:THR:HG21	1.84	1.06
1:B:509:THR:HG21	1:B:537:MET:SD	1.96	1.06
1:B:664:ASP:O	1:B:668:LYS:HG2	1.58	1.03
1:A:490:LEU:HD11	1:A:496:THR:HG21	1.40	1.00
1:B:352:LEU:HD11	1:B:425:LEU:CD1	2.01	0.91
1:A:608:ARG:O	1:A:652:ILE:HD11	1.71	0.89
1:B:352:LEU:CD1	1:B:425:LEU:HD11	2.04	0.88
1:A:490:LEU:CD1	1:A:496:THR:HG23	2.06	0.86
1:B:414:ASN:ND2	1:B:419:LEU:CB	2.36	0.82
1:B:507:ALA:HB3	1:B:508:GLY:HA2	1.62	0.81
1:A:423:SER:HB3	1:A:426:ILE:HG12	1.61	0.81
1:B:493:GLY:HA2	1:B:494:GLN:O	1.82	0.80
1:B:352:LEU:HD13	1:B:425:LEU:HD11	1.62	0.80
1:B:414:ASN:HD21	1:B:419:LEU:HB2	1.46	0.78
1:B:352:LEU:CD1	1:B:425:LEU:CD1	2.62	0.77
1:B:352:LEU:HD11	1:B:425:LEU:HD12	1.67	0.76
1:B:393:ASP:O	1:B:430:ARG:HD2	1.87	0.75
1:B:509:THR:CG2	1:B:537:MET:SD	2.75	0.75
1:A:490:LEU:HD12	1:A:496:THR:CG2	2.18	0.74
1:A:545:GLN:HG2	1:A:546:PHE:CD2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ILE:O	1:B:430:ARG:HG2	1.89	0.73
1:B:116:VAL:HG11	1:B:221:TYR:HB2	1.73	0.70
1:B:232:VAL:HB	1:B:246:TRP:HB3	1.73	0.70
1:B:126:VAL:HG13	1:B:129:ARG:CZ	2.21	0.70
1:A:119:SER:O	1:B:415:LEU:N	2.24	0.70
1:A:490:LEU:HD11	1:A:496:THR:CG2	2.07	0.69
1:B:507:ALA:N	1:B:508:GLY:HA3	2.07	0.68
1:B:505:MET:SD	1:B:560:LYS:HD3	2.35	0.67
1:B:493:GLY:HA2	1:B:494:GLN:C	2.15	0.67
1:A:114:ASP:O	1:A:118:ARG:HB2	1.95	0.67
1:A:118:ARG:O	1:B:421:GLN:NE2	2.22	0.66
1:B:388:GLN:O	1:B:389:THR:OG1	2.14	0.66
1:B:313:LEU:HA	1:B:316:MET:HE2	1.76	0.66
1:A:680:ALA:O	1:A:683:LEU:N	2.27	0.66
1:A:445:SER:OG	1:A:484:ARG:NH2	2.29	0.66
1:A:589:LEU:HD13	1:A:667:LYS:HG2	1.78	0.65
1:A:490:LEU:HD13	1:A:496:THR:HG23	1.79	0.65
1:A:376:SER:O	1:A:403:ARG:CZ	2.45	0.65
1:B:507:ALA:HB3	1:B:508:GLY:CA	2.27	0.63
1:A:490:LEU:HD12	1:A:496:THR:HG21	1.75	0.63
1:A:634:ARG:HG2	1:A:634:ARG:O	1.99	0.62
1:B:664:ASP:O	1:B:668:LYS:CG	2.43	0.62
1:B:126:VAL:CG1	1:B:129:ARG:NH2	2.62	0.62
1:B:139:LEU:HD22	1:B:156:MET:HB3	1.81	0.61
1:B:493:GLY:HA2	1:B:494:GLN:HB3	1.82	0.61
1:A:545:GLN:HG2	1:A:546:PHE:CE2	2.36	0.61
1:A:111:LYS:HE2	1:B:196:LYS:HD2	1.82	0.61
1:A:294:ASN:ND2	1:A:332:TYR:OH	2.34	0.61
1:B:238:GLU:OE1	1:B:240:ASP:N	2.32	0.60
1:B:117:ALA:O	1:B:225:MET:HG2	2.01	0.60
1:A:104:GLU:O	1:A:106:GLN:NE2	2.33	0.60
1:A:196:LYS:HD3	1:A:215:GLN:HB3	1.84	0.60
1:B:583:LYS:O	1:B:588:ARG:NH1	2.35	0.59
1:A:464:ARG:NH2	1:A:547:ASP:OD1	2.36	0.58
1:B:616:PRO:HD2	1:B:617:ARG:HG3	1.86	0.58
1:A:329:PHE:CZ	1:A:333:VAL:HG21	2.38	0.58
1:A:637:LEU:HB3	1:A:638:ARG:HA	1.86	0.58
1:B:364:LYS:NZ	1:B:458:ASP:OD1	2.33	0.58
1:A:689:ASP:OD2	1:A:707:ARG:NH2	2.26	0.58
1:A:96:VAL:HG21	1:A:100:PHE:CE1	2.39	0.58
1:A:400:ARG:O	1:A:403:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:NH2	1:A:538:GLU:OE2	2.37	0.57
1:B:689:ASP:HB3	1:B:704:MET:SD	2.44	0.57
1:A:228:ASP:OD1	1:A:273:LYS:HG2	2.04	0.57
1:A:440:PHE:O	1:A:444:GLN:HG2	2.05	0.57
1:B:337:TYR:CZ	1:B:363:MET:HE1	2.40	0.57
1:A:215:GLN:O	1:B:111:LYS:NZ	2.30	0.57
1:A:542:CYS:HB2	1:A:547:ASP:HB3	1.86	0.56
1:B:126:VAL:CG1	1:B:129:ARG:CZ	2.83	0.56
1:B:555[B]:ARG:NH2	1:B:556:GLU:OE2	2.39	0.56
1:A:512:ILE:HD11	1:A:562:LEU:HG	1.89	0.55
1:B:230:VAL:HG22	1:B:270:LEU:HD22	1.89	0.55
1:A:590:SER:OG	1:A:591:SER:N	2.40	0.54
1:A:442:LEU:HD23	1:A:482:LEU:HD23	1.89	0.54
1:A:377:SER:OG	1:A:390:LYS:HG2	2.07	0.54
1:A:490:LEU:HD13	1:A:496:THR:CG2	2.30	0.54
1:A:158:ILE:HB	1:A:300:ILE:HD13	1.89	0.54
1:A:139:LEU:HD22	1:A:156:MET:HB3	1.88	0.54
1:B:530:GLU:HA	1:B:533:LYS:HD3	1.89	0.54
1:A:512:ILE:N	1:A:561:LYS:O	2.36	0.54
1:B:470:THR:HG21	1:B:475:VAL:HB	1.90	0.54
1:A:257:ALA:HB2	1:B:100:PHE:HB3	1.88	0.54
1:A:232:VAL:HB	1:A:246:TRP:HB3	1.90	0.54
1:A:412:PRO:HD2	1:A:426:ILE:HD11	1.90	0.54
1:A:115:ILE:HG21	1:B:415:LEU:HD22	1.89	0.53
1:A:700:ASP:OD1	1:A:702:ARG:HD3	2.08	0.53
1:A:703:PRO:HA	1:B:522:LEU:HD21	1.91	0.53
1:A:545:GLN:NE2	1:A:546:PHE:CZ	2.76	0.53
1:A:554:LEU:HD23	1:A:562:LEU:HD21	1.90	0.53
1:B:414:ASN:HD22	1:B:419:LEU:HB2	1.61	0.53
1:A:546:PHE:O	1:A:550:THR:HG23	2.08	0.53
1:B:249:ASP:N	1:B:250:GLY:HA2	2.23	0.53
1:A:191:ALA:O	1:B:111:LYS:HD3	2.09	0.53
1:B:426:ILE:O	1:B:430:ARG:HG3	2.09	0.52
1:A:330:TYR:OH	1:A:361:PRO:HB3	2.09	0.52
1:A:434:GLN:NE2	1:A:475:VAL:HG21	2.24	0.52
1:A:608:ARG:O	1:A:652:ILE:CD1	2.53	0.52
1:B:190:ILE:HD13	1:B:221:TYR:CZ	2.44	0.52
1:B:518:PRO:HG2	1:B:522:LEU:HD12	1.92	0.52
1:A:673:LYS:NZ	1:A:674:ASP:OD2	2.43	0.51
1:A:483:LEU:O	1:A:484:ARG:HD3	2.11	0.51
1:A:597:LEU:HD11	1:A:669:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:GLU:OE1	1:A:699:GLU:N	2.32	0.51
1:A:316:MET:HB2	1:A:321:ILE:HD11	1.91	0.51
1:B:180:LYS:HB2	1:B:244:TYR:CZ	2.46	0.51
1:A:140:GLU:OE1	1:A:143:ARG:NH1	2.44	0.51
1:A:242:PRO:HG2	1:A:244:TYR:CZ	2.46	0.51
1:A:376:SER:O	1:A:403:ARG:NH2	2.44	0.51
1:B:299:PRO:HB3	1:B:306:ARG:CZ	2.41	0.51
1:B:352:LEU:HD22	1:B:410:ASP:OD2	2.11	0.50
1:A:511:ASN:OD1	1:A:513:TYR:CZ	2.64	0.50
1:B:232:VAL:HG22	1:B:268:ILE:HG12	1.92	0.50
1:A:230:VAL:HG22	1:A:270:LEU:HD22	1.93	0.50
1:A:598:LEU:HA	1:A:601:MET:HE2	1.94	0.49
1:A:490:LEU:HD12	1:A:496:THR:HG23	1.87	0.49
1:A:601:MET:HE3	1:A:612:ILE:HG21	1.92	0.49
1:B:605:LEU:HD23	1:B:608:ARG:HH21	1.78	0.49
1:A:546:PHE:CE1	1:B:368:PHE:HB2	2.49	0.48
1:A:701:PRO:HG2	1:B:693:ILE:HD13	1.95	0.48
1:B:633:ALA:HB1	1:B:653:LEU:HD13	1.95	0.48
1:A:180:LYS:HB2	1:A:244:TYR:CZ	2.48	0.48
1:A:528:TYR:CD1	1:A:566:GLU:HA	2.49	0.48
1:A:291:LYS:O	6:A:942:HOH:O	2.20	0.47
1:A:487:SER:OG	1:A:538:GLU:OE1	2.23	0.47
1:B:183:LEU:O	1:B:187:LEU:HB2	2.15	0.47
1:A:232:VAL:HG22	1:A:268:ILE:HG12	1.97	0.47
1:B:414:ASN:CG	1:B:419:LEU:HB2	2.26	0.47
1:B:598:LEU:HD11	1:B:614:VAL:HG23	1.95	0.47
1:B:483:LEU:O	1:B:484:ARG:NH1	2.46	0.47
1:A:635:HIS:O	1:A:639:THR:HG23	2.14	0.47
1:B:700:ASP:O	1:B:703:PRO:HD2	2.15	0.47
1:A:196:LYS:HD3	1:A:215:GLN:CB	2.44	0.46
1:A:361:PRO:HG2	1:A:459:TYR:OH	2.16	0.46
1:B:231:GLU:OE2	1:B:271:HIS:NE2	2.49	0.46
1:A:702:ARG:NH2	1:B:518:PRO:HD3	2.30	0.46
1:B:509:THR:HG21	1:B:537:MET:CE	2.46	0.46
1:A:618:LEU:HB2	1:A:660:ASN:HB2	1.98	0.45
1:A:609:VAL:HG12	1:A:655:PRO:HG2	1.98	0.45
1:A:294:ASN:ND2	1:A:332:TYR:CZ	2.84	0.45
1:A:213:ILE:HD13	1:A:385:ILE:HD11	1.98	0.45
1:B:486:GLU:CD	1:B:493:GLY:HA3	2.36	0.45
1:B:486:GLU:CD	1:B:493:GLY:H	2.20	0.45
1:B:505:MET:SD	1:B:560:LYS:CE	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:PHE:HE2	1:B:102:LYS:HE3	1.81	0.45
1:B:589:LEU:HG	1:B:667:LYS:HG2	1.99	0.45
1:B:422:GLU:O	1:B:425:LEU:HB3	2.16	0.45
1:B:493:GLY:CA	1:B:494:GLN:HB3	2.47	0.44
1:B:592:GLU:OE1	1:B:592:GLU:N	2.44	0.44
1:B:277:LYS:HD3	1:B:277:LYS:HA	1.82	0.44
1:A:478:ASP:HA	1:A:481:LYS:HE3	1.99	0.44
1:A:114:ASP:OD2	1:A:118:ARG:NH1	2.51	0.44
1:A:680:ALA:O	1:A:681:GLN:C	2.56	0.44
1:A:598:LEU:O	1:A:602:ARG:HG3	2.18	0.44
1:B:394:ILE:C	1:B:430:ARG:HG2	2.37	0.44
1:A:550:THR:O	1:A:554:LEU:N	2.50	0.44
1:B:242:PRO:HG2	1:B:244:TYR:CZ	2.52	0.44
1:B:626:THR:OG1	1:B:656:THR:HB	2.18	0.44
1:B:505:MET:SD	1:B:560:LYS:CD	3.05	0.43
1:B:517:ALA:O	1:B:543:PHE:HA	2.18	0.43
1:B:486:GLU:OE1	1:B:520:ARG:HD3	2.19	0.43
1:A:545:GLN:NE2	1:A:546:PHE:CE2	2.86	0.43
1:A:114:ASP:OD1	1:A:118:ARG:HD3	2.18	0.43
1:B:493:GLY:CA	1:B:494:GLN:C	2.86	0.43
1:A:637:LEU:CB	1:A:638:ARG:HA	2.46	0.43
1:B:693:ILE:HD11	1:B:704:MET:CE	2.48	0.43
1:A:464:ARG:HG2	1:A:550:THR:HG21	2.01	0.43
1:A:668:LYS:HA	1:A:668:LYS:HD3	1.76	0.43
1:A:396:PRO:HD2	1:A:399:LEU:HD12	2.00	0.43
1:A:199:LEU:CD2	1:A:209:SER:HA	2.50	0.42
1:A:198:PHE:CE2	1:A:202:LEU:HD11	2.55	0.42
1:A:330:TYR:CD2	1:A:340:PRO:HD3	2.54	0.42
1:B:502:SER:O	1:B:505:MET:HB2	2.19	0.42
1:A:551:LEU:HB3	1:A:562:LEU:HD23	2.02	0.42
1:B:531:ALA:O	1:B:617:ARG:NH2	2.49	0.41
1:B:186:ASN:HB3	3:B:803:ADP:H4'	2.01	0.41
1:B:489:ALA:O	1:B:490:LEU:HD23	2.21	0.41
1:B:172:GLN:HA	1:B:266:THR:O	2.20	0.41
1:B:178:MET:N	1:B:234:SER:OG	2.53	0.41
1:A:289:VAL:HG11	1:A:307:LEU:HD12	2.02	0.41
1:B:290:THR:O	1:B:294:ASN:HB2	2.21	0.41
1:A:467:ILE:HD12	1:A:483:LEU:HD11	2.01	0.41
1:B:227:ALA:HB2	1:B:270:LEU:HB3	2.03	0.41
1:A:252:GLY:O	1:B:104:GLU:HG3	2.20	0.41
1:B:411:ILE:CG2	1:B:420:LEU:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASP:OD1	1:A:277:LYS:NZ	2.51	0.41
1:B:615:THR:HA	1:B:616:PRO:HD3	1.93	0.40
1:B:366:SER:HB3	1:B:369:ASP:HB2	2.02	0.40
1:B:492:ALA:O	1:B:494:GLN:HB2	2.21	0.40
1:A:420:LEU:HD13	1:A:426:ILE:HD12	2.04	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	584/647 (90%)	551 (94%)	32 (6%)	1 (0%)	52	63
1	B	601/647 (93%)	572 (95%)	28 (5%)	1 (0%)	52	63
All	All	1185/1294 (92%)	1123 (95%)	60 (5%)	2 (0%)	52	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	491	PRO
1	A	150	GLY

### 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	520/569 (91%)	516 (99%)	4 (1%)	86	94
1	B	543/569 (95%)	540 (99%)	3 (1%)	90	96
All	All	1063/1138 (93%)	1056 (99%)	7 (1%)	88	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	119	SER
1	A	126	VAL
1	A	215	GLN
1	B	155	PRO
1	B	394	ILE
1	B	606	VAL

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	294	ASN
1	B	161	GLN
1	B	235	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ADP	A	803	5,4	22,29,29	1.06	1 (4%)	27,45,45	1.87	5 (18%)
4	BEF	A	804	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	B	803	5,4	22,29,29	1.05	2 (9%)	27,45,45	2.05	6 (22%)
4	BEF	B	804	3	0,3,3	0.00	-	0,3,3	0.00	-

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	ADP	A	803	5,4	-	0/12/32/32	0/3/3/3
4	BEF	A	804	3	-	0/0/0/0	0/0/0/0
3	ADP	B	803	5,4	-	0/12/32/32	0/3/3/3
4	BEF	B	804	3	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	ADP	O4'-C1'	2.08	1.43	1.41
3	A	803	ADP	C5-C4	3.24	1.47	1.40
3	B	803	ADP	C5-C4	3.26	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	ADP	N3-C2-N1	-7.35	123.27	128.89
3	A	803	ADP	N3-C2-N1	-7.28	123.32	128.89
3	B	803	ADP	C2'-C1'-N9	-3.69	108.66	114.29
3	B	803	ADP	PA-O3A-PB	-3.64	120.46	132.67
3	B	803	ADP	C4-C5-N7	-3.02	106.70	109.48
3	A	803	ADP	C2'-C1'-N9	-2.88	109.90	114.29
3	A	803	ADP	PA-O3A-PB	-2.39	124.65	132.67
3	A	803	ADP	C4-C5-N7	-2.16	107.49	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	ADP	C2-N1-C6	2.24	122.77	118.77
3	B	803	ADP	O3B-PB-O2B	2.41	116.56	107.38
3	A	803	ADP	C2-N1-C6	2.46	123.17	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	ADP	1	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	594/647 (91%)	0.76	69 (11%) 6 11	26, 79, 140, 185	0
1	B	609/647 (94%)	0.48	35 (5%) 27 41	50, 74, 124, 154	0
All	All	1203/1294 (92%)	0.62	104 (8%) 13 21	26, 76, 136, 185	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	PHE	9.2
1	A	374	MET	8.5
1	A	677	PRO	7.9
1	A	508	GLY	7.4
1	A	609	VAL	6.5
1	A	324	TRP	6.2
1	A	529	PHE	5.8
1	A	716	LEU	5.7
1	A	597	LEU	5.6
1	A	679	LEU	5.3
1	B	607	GLN	5.2
1	B	652	ILE	5.2
1	B	653	LEU	5.0
1	A	607	GLN	4.9
1	B	352	LEU	4.4
1	A	151	GLY	4.4
1	A	589	LEU	4.2
1	A	394	ILE	4.2
1	B	147	ILE	4.2
1	A	617	ARG	4.0
1	A	531	ALA	3.9
1	A	666	ILE	3.9
1	A	613	LYS	3.9
1	A	99	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	670	HIS	3.8
1	A	628	LEU	3.6
1	A	605	LEU	3.6
1	B	699	GLU	3.6
1	B	146	MET	3.5
1	B	238	GLU	3.3
1	A	638	ARG	3.3
1	B	126	VAL	3.2
1	A	598	LEU	3.2
1	B	636	PHE	3.2
1	A	533	LYS	3.2
1	A	671	ALA	3.2
1	A	391	ALA	3.2
1	B	149	ALA	3.1
1	A	530	GLU	3.1
1	A	672	LEU	3.1
1	A	684	LEU	3.0
1	B	586	SER	3.0
1	A	665	LEU	3.0
1	A	718	LYS	2.9
1	A	600	TRP	2.9
1	B	576	GLU	2.9
1	A	555	ARG	2.9
1	A	659	ILE	2.9
1	A	150	GLY	2.9
1	A	612	ILE	2.9
1	A	498	LEU	2.9
1	A	712	LEU	2.9
1	B	252	GLY	2.8
1	A	687	ILE	2.8
1	A	604	ALA	2.8
1	A	537	MET	2.8
1	B	415	LEU	2.8
1	A	634	ARG	2.8
1	B	413	LEU	2.8
1	A	606	VAL	2.7
1	A	120	LEU	2.7
1	A	678	GLU	2.7
1	A	153	THR	2.7
1	A	708	LEU	2.7
1	B	240	ASP	2.7
1	B	269	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	233	TYR	2.6
1	A	601	MET	2.6
1	A	608	ARG	2.6
1	B	148	THR	2.6
1	A	669	LEU	2.5
1	A	682	LEU	2.5
1	A	592	GLU	2.5
1	A	97	GLN	2.5
1	A	90	ILE	2.4
1	B	236	SER	2.4
1	B	102	LYS	2.4
1	B	425	LEU	2.4
1	B	110	LYS	2.4
1	A	98	GLY	2.3
1	B	232	VAL	2.3
1	A	668	LYS	2.3
1	A	117	ALA	2.3
1	B	384	LYS	2.3
1	A	145	ARG	2.3
1	B	239	ALA	2.3
1	B	389	THR	2.3
1	B	510	ARG	2.2
1	A	214	GLY	2.2
1	A	618	LEU	2.2
1	B	505	MET	2.2
1	A	540	LEU	2.2
1	A	567	THR	2.2
1	A	594	ALA	2.2
1	A	528	TYR	2.2
1	B	666	ILE	2.2
1	B	165	VAL	2.2
1	A	683	LEU	2.1
1	B	363	MET	2.1
1	B	257	ALA	2.1
1	A	652	ILE	2.1
1	B	429	LEU	2.0
1	A	471	GLY	2.0
1	A	393	ASP	2.0

## 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 [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
5	MG	A	805	1/1	0.93	0.23	0.88	51,51,51,51	0
4	BEF	B	804	4/4	0.99	0.21	0.67	52,57,58,77	0
5	MG	B	805	1/1	0.99	0.19	0.35	49,49,49,49	0
4	BEF	A	804	4/4	0.99	0.20	-0.14	34,41,41,44	0
3	ADP	A	803	27/27	0.98	0.18	-0.27	39,48,55,57	0
3	ADP	B	803	27/27	0.98	0.15	-0.29	51,60,68,75	0
2	CO	B	802	1/1	0.96	0.35	-	109,109,109,109	1
2	CO	B	801	1/1	0.94	0.18	-	94,94,94,94	0
2	CO	A	802	1/1	0.61	0.14	-	113,113,113,113	1
2	CO	A	801	1/1	0.90	0.11	-	109,109,109,109	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.