



Full wwPDB X-ray Structure Validation Report

Aug 20, 2014 – 10:44 AM EDT

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 validation 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>

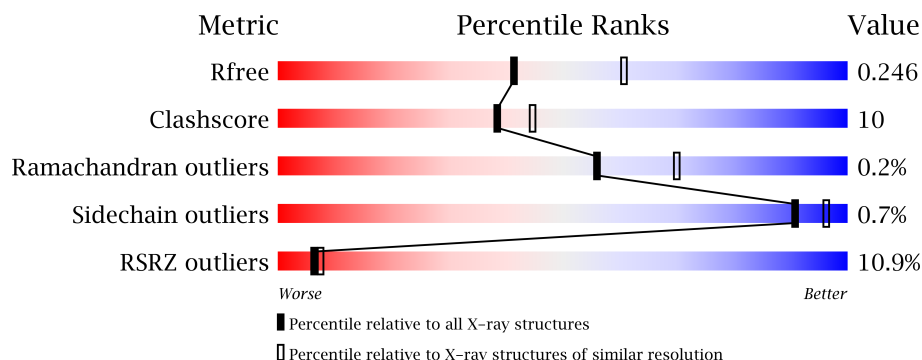
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

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}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	647	
1	B	647	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	CO	A	802	-	X
2	CO	B	802	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 9953 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.

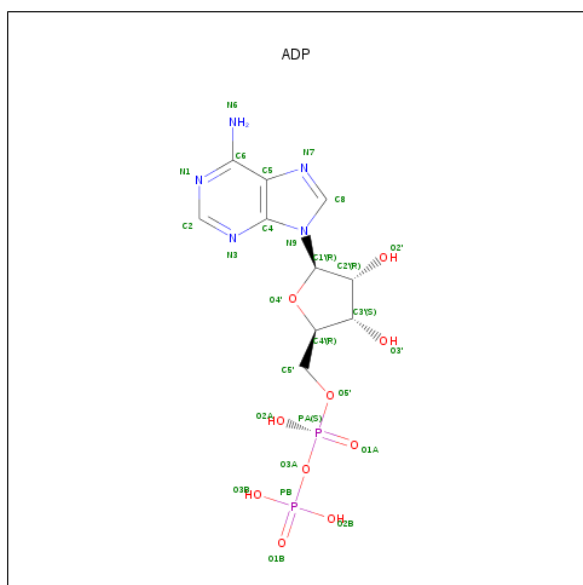
- Molecule 1 is a protein called TNF receptor-associated protein 1.

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).

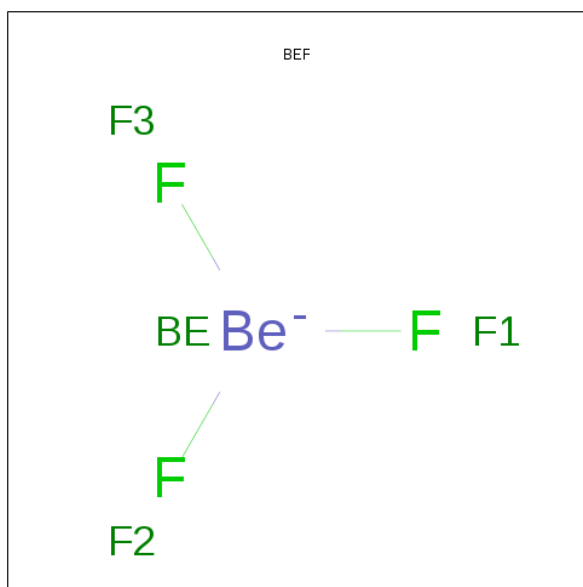
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Co	0	0
			2	2		
2	A	2	Total	Co	0	0
			2	2		

- 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: BeF₃).



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		

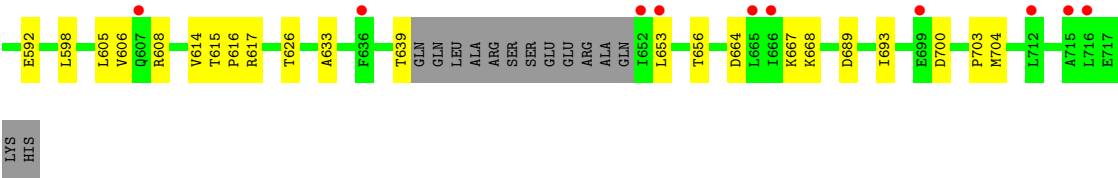
- Molecule 6 is water.

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

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.78Å 96.57Å 124.98Å 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
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1278)	Depositor
R, R_{free}	0.205 , 0.248 0.210 , 0.246	Depositor DCC
R_{free} test set	1852 reflections (3.24%)	DCC
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.1	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	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: 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 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	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

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 10.

All (191) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:680:ALA:O	1:A:683:LEU:N	2.27	0.66
1:B:313:LEU:HA	1:B:316:MET:HE2	1.76	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:A:689:ASP:OD2	1:A:707:ARG:NH2	2.26	0.58
1:B:364:LYS:NZ	1:B:458:ASP:OD1	2.33	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:377:SER:OG	1:A:390:LYS:HG2	2.07	0.54
1:A:442:LEU:HD23	1:A:482:LEU:HD23	1.89	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:232:VAL:HB	1:A:246:TRP:HB3	1.90	0.54
1:A:257:ALA:HB2	1:B:100:PHE:HB3	1.88	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:A:546:PHE:O	1:A:550:THR:HG23	2.08	0.53
1:B:414:ASN:HD22	1:B:419:LEU:HB2	1.61	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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:A:511:ASN:OD1	1:A:513:TYR:CZ	2.64	0.50
1:B:352:LEU:HD22	1:B:410:ASP:OD2	2.11	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:A:635:HIS:O	1:A:639:THR:HG23	2.14	0.47
1:B:483:LEU:O	1:B:484:ARG:NH1	2.46	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:100:PHE:HE2	1:B:102:LYS:HE3	1.81	0.45
1:B:505:MET:SD	1:B:560:LYS:CE	3.04	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:N	1:B:592:GLU:OE1	2.44	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:598:LEU:O	1:A:602:ARG:HG3	2.18	0.44
1:A:680:ALA:O	1:A:681:GLN:C	2.56	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:394:ILE:C	1:B:430:ARG:HG2	2.37	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:114:ASP:OD1	1:A:118:ARG:HD3	2.18	0.43
1:A:545:GLN:NE2	1:A:546:PHE:CE2	2.86	0.43
1:A:637:LEU:CB	1:A:638:ARG:HA	2.46	0.43
1:B:493:GLY:CA	1:B:494:GLN:C	2.86	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:186:ASN:HB3	3:B:803:ADP:H4'	2.01	0.41
1:B:531:ALA:O	1:B:617:ARG:NH2	2.49	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:A:289:VAL:HG11	1:A:307:LEU:HD12	2.02	0.41
1:B:178:MET:N	1:B:234:SER:OG	2.53	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:274:ASP:OD1	1:A:277:LYS:NZ	2.51	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
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

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	584/647 (90%)	551 (94%)	32 (6%)	1 (0%)	56	70
1	B	601/647 (93%)	572 (95%)	28 (5%)	1 (0%)	56	70
All	All	1185/1294 (92%)	1123 (95%)	60 (5%)	2 (0%)	56	70

All (2) Ramachandran outliers are listed below:

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

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	520/569 (91%)	516 (99%)	4 (1%)	89	95
1	B	543/569 (95%)	540 (99%)	3 (1%)	92	97
All	All	1063/1138 (93%)	1056 (99%)	7 (1%)	91	96

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

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Mol	Chain	Res	Type
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 ⓘ

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 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	29,29,29	1.21	2 (6%)	45,45,45	2.01	8 (17%)
4	BEF	A	804	3	0,3,3	0.00	-	0,3,3	0.00	-
3	ADP	B	803	5,4	29,29,29	1.11	3 (10%)	45,45,45	2.12	9 (20%)
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	-	0/16/32/32	0/3/3/3
4	BEF	A	804	3	-	0/0/0/0	0/0/0/0
3	ADP	B	803	5,4	-	0/16/32/32	0/3/3/3
4	BEF	B	804	3	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	ADP	C5-C4	3.26	1.47	1.40
3	A	803	ADP	C5-C4	3.24	1.47	1.40
3	A	803	ADP	C4-N9	-2.94	1.33	1.37
3	B	803	ADP	C4-N9	-2.83	1.33	1.37
3	B	803	ADP	O4'-C1'	2.08	1.43	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	ADP	C5-C4-N3	-7.52	118.65	125.98
3	A	803	ADP	C5-C4-N3	-6.54	119.60	125.98
3	B	803	ADP	N3-C2-N1	-6.39	123.27	128.89
3	A	803	ADP	N3-C2-N1	-6.33	123.32	128.89
3	A	803	ADP	N3-C4-N9	5.81	135.36	125.39
3	B	803	ADP	N3-C4-N9	5.56	134.92	125.39
3	B	803	ADP	PA-O3A-PB	-4.14	120.46	131.93
3	A	803	ADP	C8-N9-C4	3.10	109.48	106.96
3	B	803	ADP	C4-C5-N7	-2.81	106.70	109.41
3	B	803	ADP	C2-N3-C4	2.66	120.93	113.27
3	A	803	ADP	PA-O3A-PB	-2.63	124.65	131.93
3	B	803	ADP	C3'-C2'-C1'	2.60	105.00	100.92
3	A	803	ADP	C2-N1-C6	2.48	123.17	118.76
3	B	803	ADP	O3B-PB-O2B	2.45	116.56	107.38
3	A	803	ADP	C2-N3-C4	2.31	119.93	113.27
3	B	803	ADP	C2-N1-C6	2.25	122.77	118.76
3	A	803	ADP	C3'-C2'-C1'	2.16	104.31	100.92

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	594/647 (91%)	0.82	79 (13%) 4 5	26, 79, 140, 185	0
1	B	609/647 (94%)	0.55	52 (8%) 11 13	50, 74, 124, 154	0
All	All	1203/1294 (92%)	0.68	131 (10%) 6 7	26, 76, 136, 185	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	MET	12.0
1	A	100	PHE	10.0
1	A	716	LEU	7.8
1	A	677	PRO	7.5
1	A	679	LEU	6.3
1	A	609	VAL	6.2
1	A	394	ILE	6.1
1	A	508	GLY	5.7
1	B	653	LEU	5.6
1	B	607	GLN	5.5
1	A	529	PHE	5.4
1	A	607	GLN	5.3
1	A	324	TRP	5.3
1	B	147	ILE	5.3
1	B	352	LEU	5.3
1	A	597	LEU	5.2
1	A	672	LEU	4.6
1	A	712	LEU	4.5
1	B	252	GLY	4.4
1	B	652	ILE	4.4
1	A	628	LEU	4.4
1	A	99	SER	4.4
1	B	149	ALA	4.3
1	B	209	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	391	ALA	4.2
1	B	716	LEU	4.1
1	B	146	MET	4.0
1	A	589	LEU	4.0
1	A	670	HIS	3.9
1	A	665	LEU	3.9
1	A	605	LEU	3.8
1	A	666	ILE	3.8
1	A	671	ALA	3.6
1	A	683	LEU	3.6
1	A	669	LEU	3.5
1	A	531	ALA	3.5
1	A	617	ARG	3.4
1	A	604	ALA	3.4
1	A	600	TRP	3.4
1	A	718	LYS	3.4
1	B	636	PHE	3.4
1	B	429	LEU	3.3
1	A	120	LEU	3.2
1	A	684	LEU	3.2
1	B	253	VAL	3.2
1	A	393	ASP	3.2
1	A	151	GLY	3.2
1	B	232	VAL	3.2
1	B	269	VAL	3.2
1	B	233	TYR	3.1
1	A	632	ALA	3.1
1	A	638	ARG	3.1
1	B	413	LEU	3.1
1	B	351	PRO	3.1
1	B	420	LEU	3.1
1	B	102	LYS	3.1
1	A	601	MET	3.1
1	A	613	LYS	3.1
1	A	708	LEU	3.0
1	A	668	LYS	3.0
1	A	153	THR	3.0
1	A	537	MET	3.0
1	B	126	VAL	3.0
1	B	415	LEU	2.9
1	B	699	GLU	2.9
1	B	715	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	498	LEU	2.9
1	B	148	THR	2.9
1	B	586	SER	2.9
1	A	395	LEU	2.9
1	A	429	LEU	2.9
1	B	576	GLU	2.8
1	A	652	ILE	2.8
1	A	555	ARG	2.8
1	B	249	ASP	2.8
1	A	97	GLN	2.8
1	B	220	PHE	2.7
1	A	598	LEU	2.7
1	B	384	LYS	2.7
1	B	389	THR	2.7
1	A	117	ALA	2.7
1	A	98	GLY	2.7
1	B	712	LEU	2.6
1	B	187	LEU	2.6
1	B	425	LEU	2.6
1	A	687	ILE	2.6
1	A	541	PHE	2.6
1	B	246	TRP	2.6
1	B	119	SER	2.6
1	A	608	ARG	2.6
1	A	612	ILE	2.5
1	B	110	LYS	2.5
1	A	217	GLY	2.5
1	B	211	SER	2.5
1	A	530	GLU	2.4
1	A	533	LYS	2.4
1	A	634	ARG	2.4
1	A	96	VAL	2.4
1	B	510	ARG	2.4
1	A	606	VAL	2.4
1	A	636	PHE	2.4
1	B	144	HIS	2.4
1	B	165	VAL	2.3
1	A	678	GLU	2.3
1	A	145	ARG	2.3
1	A	639	THR	2.3
1	B	665	LEU	2.3
1	B	666	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	256	VAL	2.2
1	A	592	GLU	2.2
1	B	231	GLU	2.2
1	A	214	GLY	2.2
1	A	406	VAL	2.2
1	A	528	TYR	2.2
1	B	113	LEU	2.1
1	A	150	GLY	2.1
1	A	567	THR	2.1
1	A	711	LEU	2.1
1	B	374	MET	2.1
1	A	630	MET	2.1
1	B	363	MET	2.1
1	A	471	GLY	2.1
1	A	629	GLU	2.1
1	B	335	GLN	2.1
1	B	580	GLN	2.1
1	B	224	PHE	2.1
1	B	358	PHE	2.1
1	A	112	LEU	2.0
1	A	190	ILE	2.0
1	B	305	ARG	2.0
1	A	594	ALA	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 ⓘ

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(\AA^2)	Q<0.9
2	CO	B	802	1/1	0.34	9.61	109,109,109,109	1
2	CO	A	802	1/1	0.13	2.26	113,113,113,113	1
5	MG	A	805	1/1	0.25	1.00	51,51,51,51	0
4	BEF	B	804	4/4	0.23	0.93	52,57,58,77	0
4	BEF	A	804	4/4	0.23	0.11	34,41,41,44	0
5	MG	B	805	1/1	0.19	-0.03	49,49,49,49	0
3	ADP	A	803	27/27	0.19	-0.07	39,48,55,57	0
2	CO	B	801	1/1	0.18	-0.09	94,94,94,94	0
3	ADP	B	803	27/27	0.15	-0.31	51,60,68,75	0
2	CO	A	801	1/1	0.11	-1.53	109,109,109,109	1

6.5 Other polymers ⓘ

There are no such residues in this entry.