Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:52 PM GMT

PDB ID : 1R10
Title : Cystic fibrosis transmembrane conductance regulator (CFTR) nucleotide-binding domain one (NBD1) with ATP, I4122 space group
Authors : Lewis, H.A.; Buchanan, S.G.; Burley, S.K.; Conners, K.; Dickey, M.; Dorwart, M.; Fowler, R.; Gao, X.; Guggino, W.B.; Hendrickson, W.A.
Deposited on : 2003-09-23
Resolution : 3.00 Å(reported)

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
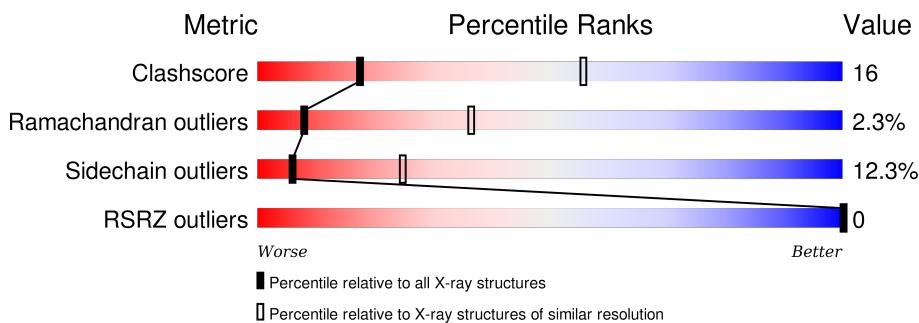
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
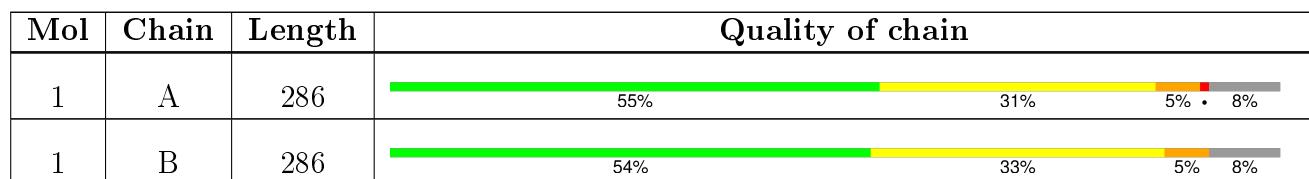
The reported resolution of this entry is 3.00 Å.

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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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 <=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	286	55% / 31% / 5% · 8%
1	B	286	54% / 33% / 5% 8%

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	ACY	A	7	-	-	X	X
4	ACY	A	9	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	B	8	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4240 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 Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2082	1327	344	399	12			
1	B	264	Total	C	N	O	S	0	0	0
			2082	1327	344	399	12			
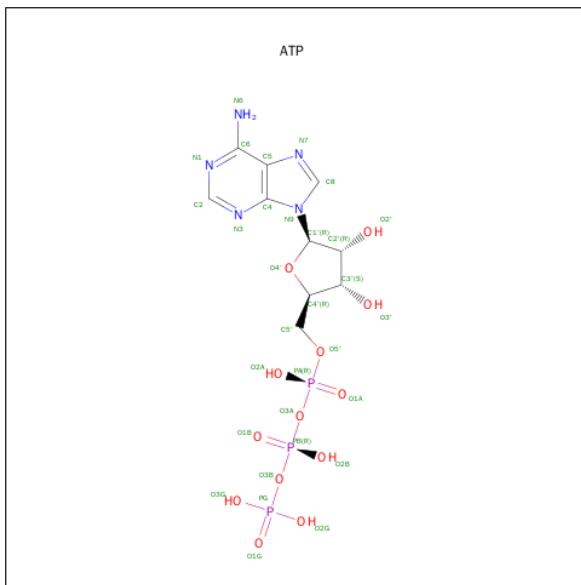
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	CLONING ARTIFACT	UNP P26361
B	388	SER	-	CLONING ARTIFACT	UNP P26361

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).
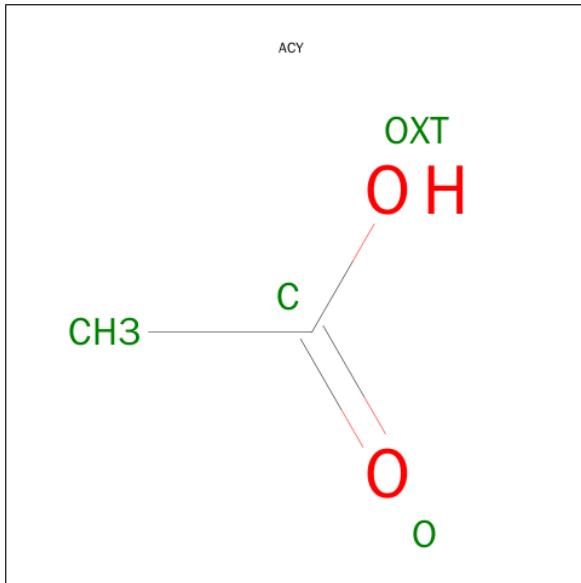
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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

ATP

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 ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).

ACY

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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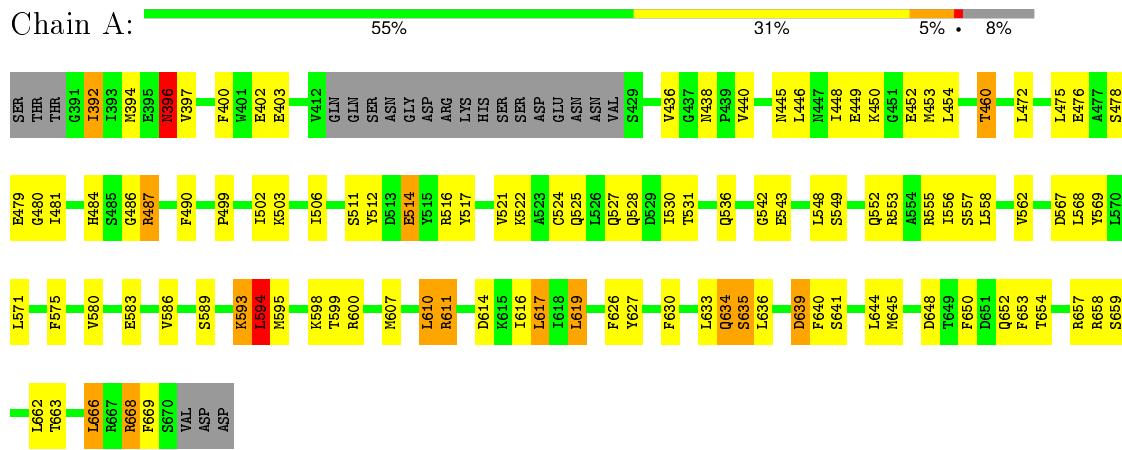
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
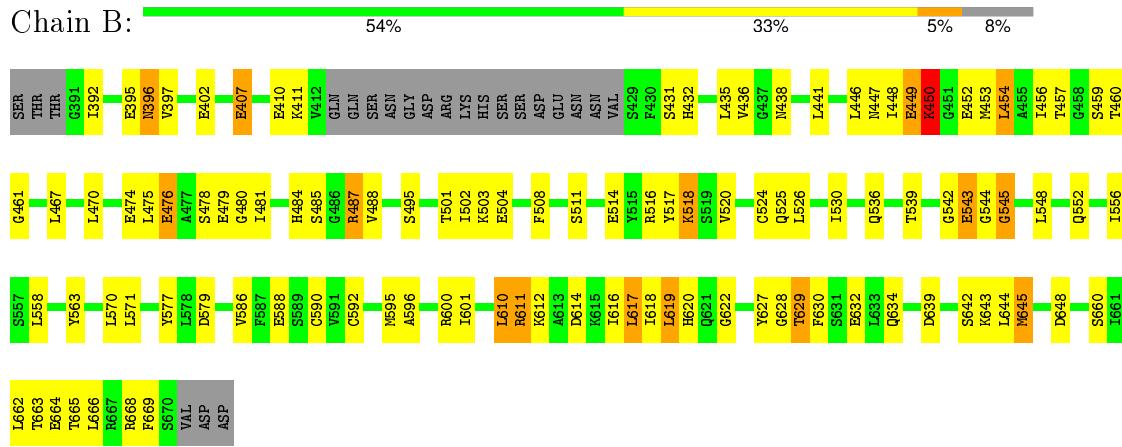
3 Residue-property plots ⓘ

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: Cystic fibrosis transmembrane conductance regulator

- Molecule 1: Cystic fibrosis transmembrane conductance regulator

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	141.20Å 141.20Å 279.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 99.9 (49.66-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.228 , 0.265 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å²)	88.9	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Outliers	0 of 28541 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4240	wwPDB-VP
Average B, all atoms (Å²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ACY, 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	0.52	0/2117	0.63	1/2846 (0.0%)
1	B	0.58	0/2117	0.69	0/2846
All	All	0.55	0/4234	0.66	1/5692 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	ARG	NE-CZ-NH1	-5.11	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	579	ASP	Peptide

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	2082	0	2081	65	0
1	B	2082	0	2081	70	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	8	0	6	2	0
4	B	4	0	3	0	0
All	All	4240	0	4195	135	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 16.

All (135) 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:392:ILE:HD12	1:B:484:HIS:HB3	1.42	1.00
1:A:516:ARG:HH11	1:A:516:ARG:HG3	1.37	0.89
1:B:501:THR:OG1	1:B:504:GLU:HG3	1.73	0.88
1:B:456:ILE:HD13	1:B:467:LEU:HD23	1.62	0.78
1:A:542:GLY:H	4:A:7:ACY:H2	1.51	0.75
1:A:610:LEU:HG	1:A:616:ILE:HD13	1.73	0.71
1:B:476:GLU:H	1:B:476:GLU:CD	1.93	0.71
1:B:396:ASN:O	1:B:480:GLY:HA3	1.91	0.71
1:B:392:ILE:HG22	1:B:448:ILE:HB	1.75	0.69
1:B:407:GLU:HG3	1:B:411:LYS:HE2	1.74	0.68
1:A:516:ARG:NH1	1:A:516:ARG:HG3	2.08	0.68
1:A:575:PHE:HD1	1:A:583:GLU:HG2	1.58	0.66
1:B:610:LEU:HG	1:B:616:ILE:HD13	1.76	0.66
1:B:668:ARG:NH2	1:B:669:PHE:HZ	1.95	0.65
1:B:525:GLN:HG2	1:B:586:VAL:HG22	1.79	0.65
1:B:644:LEU:HD11	1:B:662:LEU:HD23	1.78	0.65
1:B:530:ILE:O	1:B:536:GLN:HA	1.98	0.64
1:A:440:VAL:HG11	1:A:475:LEU:HD21	1.79	0.63
1:A:452:GLU:HA	1:A:614:ASP:OD2	1.99	0.62
1:B:617:LEU:HD22	1:B:619:LEU:HD13	1.83	0.61
1:B:432:HIS:O	1:B:436:VAL:HG23	2.01	0.61
1:A:549:SER:OG	1:A:552:GLN:HG3	2.00	0.60
1:A:611:ARG:HG3	1:A:630:PHE:CE2	2.36	0.60
1:B:452:GLU:HA	1:B:614:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LEU:HD22	1:A:619:LEU:CD1	2.31	0.60
1:A:499:PRO:HD3	1:A:543:GLU:HG2	1.83	0.60
1:A:402:GLU:HG3	1:A:476:GLU:CD	2.21	0.60
1:B:525:GLN:HG2	1:B:586:VAL:CG2	2.33	0.59
1:B:470:LEU:HD12	1:B:475:LEU:O	2.03	0.59
1:A:400:PHE:HD2	1:A:478:SER:HG	1.51	0.59
1:B:456:ILE:CD1	1:B:467:LEU:HD23	2.33	0.58
1:B:474:GLU:OE2	1:B:474:GLU:HA	2.03	0.58
1:B:668:ARG:NH2	1:B:669:PHE:CZ	2.73	0.57
1:B:392:ILE:CG2	1:B:448:ILE:HB	2.34	0.56
1:A:394:MET:HB2	1:A:446:LEU:HG	1.87	0.56
1:A:542:GLY:H	4:A:7:ACY:CH3	2.17	0.56
1:A:668:ARG:HG2	1:A:669:PHE:CE1	2.40	0.56
1:B:630:PHE:O	1:B:634:GLN:HG3	2.06	0.56
1:A:525:GLN:HG2	1:A:586:VAL:HG22	1.87	0.56
1:B:446:LEU:HA	1:B:627:TYR:CE2	2.43	0.54
1:A:552:GLN:O	1:A:556:ILE:HG13	2.08	0.53
1:B:459:SER:HB3	1:B:620:HIS:ND1	2.23	0.53
1:B:453:MET:HB2	1:B:600:ARG:CZ	2.38	0.53
1:B:487:ARG:CZ	1:B:487:ARG:HB2	2.39	0.52
1:A:402:GLU:HG3	1:A:476:GLU:OE1	2.10	0.52
1:A:594:LEU:HG	1:A:594:LEU:O	2.08	0.52
1:A:530:ILE:O	1:A:536:GLN:HA	2.09	0.52
1:A:486:GLY:HA3	1:A:567:ASP:OD2	2.10	0.51
1:A:503:LYS:NZ	1:A:512:TYR:HE1	2.08	0.51
1:B:563:TYR:CD2	1:B:563:TYR:O	2.63	0.51
1:A:644:LEU:HD21	1:A:662:LEU:CD2	2.40	0.51
1:B:544:GLY:O	1:B:545:GLY:C	2.49	0.51
1:B:449:GLU:HG3	1:B:452:GLU:OE1	2.11	0.51
1:A:460:THR:HG23	1:A:663:THR:OG1	2.11	0.51
1:A:453:MET:HG2	1:A:600:ARG:HG3	1.94	0.50
1:A:436:VAL:HG12	1:A:438:ASN:OD1	2.10	0.50
1:B:514:GLU:O	1:B:518:LYS:HB2	2.12	0.50
1:A:569:TYR:HE1	1:A:598:LYS:HD2	1.76	0.49
1:B:503:LYS:HG3	1:B:517:TYR:CZ	2.47	0.49
1:B:459:SER:HB2	1:B:663:THR:HG23	1.93	0.49
1:B:461:GLY:O	3:B:2:ATP:H3'	2.13	0.49
1:A:525:GLN:HB3	1:A:528:GLN:HE22	1.77	0.49
1:A:392:ILE:HD12	1:A:484:HIS:HB3	1.94	0.49
1:A:516:ARG:CG	1:A:516:ARG:HH11	2.17	0.49
1:A:626:PHE:CE2	1:A:633:LEU:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:N	1:A:445:ASN:OD1	2.42	0.49
1:B:524:CYS:O	1:B:525:GLN:HB2	2.13	0.49
1:A:487:ARG:HB2	1:A:487:ARG:CZ	2.42	0.49
1:B:629:THR:HG23	1:B:632:GLU:OE2	2.13	0.48
1:B:644:LEU:HD11	1:B:662:LEU:CD2	2.42	0.48
1:B:449:GLU:O	1:B:450:LYS:C	2.51	0.48
1:B:446:LEU:HD22	1:B:454:LEU:HD11	1.95	0.48
1:A:607:MET:HA	1:A:607:MET:HE2	1.95	0.48
1:B:460:THR:HG22	1:B:663:THR:OG1	2.13	0.48
1:B:590:CYS:O	1:B:595:MET:HB2	2.12	0.48
1:B:592:CYS:O	1:B:596:ALA:HB2	2.13	0.48
1:B:449:GLU:O	1:B:452:GLU:HB2	2.13	0.47
1:A:392:ILE:CG2	1:A:448:ILE:HB	2.44	0.47
1:B:611:ARG:NH1	1:B:645:MET:HE2	2.28	0.47
1:B:396:ASN:O	1:B:480:GLY:CA	2.62	0.47
1:B:502:ILE:HG23	1:B:556:ILE:HD13	1.96	0.47
1:A:593:LYS:O	1:A:595:MET:N	2.48	0.47
1:A:641:SER:O	1:A:645:MET:HB2	2.15	0.47
1:B:542:GLY:O	1:B:543:GLU:O	2.33	0.47
1:A:524:CYS:O	1:A:555:ARG:HD2	2.14	0.47
1:A:503:LYS:HZ1	1:A:512:TYR:HE1	1.63	0.46
1:A:396:ASN:HD22	1:A:445:ASN:HD21	1.63	0.46
1:B:407:GLU:OE1	1:B:411:LYS:HG3	2.15	0.46
1:B:610:LEU:HG	1:B:616:ILE:CD1	2.44	0.46
1:A:617:LEU:HD22	1:A:619:LEU:HD12	1.96	0.46
1:B:457:THR:CG2	1:B:618:ILE:HG12	2.47	0.45
1:A:568:LEU:HD12	1:A:599:THR:O	2.16	0.45
1:A:396:ASN:O	1:A:480:GLY:CA	2.64	0.45
1:B:392:ILE:CD1	1:B:484:HIS:HB3	2.30	0.45
1:A:440:VAL:CG1	1:A:475:LEU:HD21	2.45	0.45
1:B:484:HIS:ND1	1:B:485:SER:N	2.64	0.45
1:B:542:GLY:O	1:B:545:GLY:N	2.49	0.44
1:A:527:GLN:O	1:A:531:THR:HG22	2.15	0.44
1:A:397:VAL:HA	1:A:480:GLY:HA3	1.98	0.44
1:A:666:LEU:HD13	1:A:666:LEU:HA	1.71	0.44
1:B:397:VAL:HA	1:B:479:GLU:O	2.18	0.44
1:B:643:LYS:HD3	1:B:665:THR:OG1	2.18	0.44
1:B:639:ASP:HB3	1:B:669:PHE:CE2	2.52	0.44
1:A:517:TYR:CE2	1:A:521:VAL:HG21	2.53	0.44
1:B:552:GLN:O	1:B:556:ILE:HG13	2.17	0.43
1:B:453:MET:HA	1:B:600:ARG:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:GLY:O	1:B:543:GLU:C	2.56	0.43
1:A:644:LEU:HD21	1:A:662:LEU:HD21	2.00	0.43
1:A:512:TYR:OH	1:A:514:GLU:HG2	2.19	0.43
1:B:402:GLU:HG2	1:B:476:GLU:OE1	2.19	0.43
1:A:626:PHE:CD1	1:A:627:TYR:N	2.87	0.43
1:A:654:THR:O	1:A:658:ARG:HG3	2.18	0.43
1:A:472:LEU:HD11	1:A:490:PHE:CD2	2.53	0.43
1:B:627:TYR:CD1	1:B:628:GLY:N	2.87	0.42
1:A:400:PHE:HD2	1:A:478:SER:OG	2.02	0.42
1:B:501:THR:HA	1:B:539:THR:O	2.19	0.42
1:A:502:ILE:O	1:A:506:ILE:HG13	2.20	0.42
1:B:526:LEU:O	1:B:530:ILE:HG12	2.19	0.42
1:B:660:SER:O	1:B:664:GLU:HG3	2.20	0.42
1:A:525:GLN:HB3	1:A:528:GLN:NE2	2.34	0.41
1:B:441:LEU:HA	1:B:622:GLY:O	2.20	0.41
1:A:562:VAL:HG22	1:A:595:MET:CE	2.50	0.41
1:A:580:VAL:HG21	1:A:652:GLN:HA	2.02	0.41
1:A:635:SER:OG	1:A:636:LEU:N	2.53	0.41
1:B:588:GLU:O	1:B:592:CYS:HB2	2.20	0.41
1:A:650:PHE:HA	1:A:653:PHE:CD1	2.56	0.41
1:B:617:LEU:HD22	1:B:619:LEU:CD1	2.50	0.41
1:B:570:LEU:CD2	1:B:601:ILE:HD12	2.50	0.41
1:A:639:ASP:HB3	1:A:669:PHE:CE2	2.56	0.40
1:A:449:GLU:O	1:A:452:GLU:HG3	2.21	0.40
1:A:503:LYS:HE3	1:A:512:TYR:CE1	2.56	0.40
1:B:481:ILE:HD12	1:B:481:ILE:HA	1.89	0.40
1:B:516:ARG:O	1:B:520:VAL:HG23	2.21	0.40
1:B:577:TYR:CD2	1:B:577:TYR:N	2.88	0.40
1:A:634:GLN:HE21	1:A:634:GLN:HB2	1.56	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	260/286 (91%)	232 (89%)	23 (9%)	5 (2%)	10	43
1	B	260/286 (91%)	237 (91%)	16 (6%)	7 (3%)	6	32
All	All	520/572 (91%)	469 (90%)	39 (8%)	12 (2%)	8	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	543	GLU
1	A	396	ASN
1	A	648	ASP
1	B	508	PHE
1	A	594	LEU
1	A	640	PHE
1	B	396	ASN
1	B	450	LYS
1	B	545	GLY
1	B	611	ARG
1	A	593	LYS
1	B	612	LYS

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	231/252 (92%)	202 (87%)	29 (13%)	5	24
1	B	231/252 (92%)	203 (88%)	28 (12%)	6	25
All	All	462/504 (92%)	405 (88%)	57 (12%)	6	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ILE
1	A	396	ASN
1	A	403	GLU
1	A	450	LYS

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Mol	Chain	Res	Type
1	A	454	LEU
1	A	460	THR
1	A	479	GLU
1	A	481	ILE
1	A	487	ARG
1	A	511	SER
1	A	514	GLU
1	A	522	LYS
1	A	548	LEU
1	A	557	SER
1	A	558	LEU
1	A	571	LEU
1	A	589	SER
1	A	594	LEU
1	A	610	LEU
1	A	611	ARG
1	A	617	LEU
1	A	619	LEU
1	A	634	GLN
1	A	635	SER
1	A	639	ASP
1	A	657	ARG
1	A	659	SER
1	A	666	LEU
1	A	668	ARG
1	B	395	GLU
1	B	407	GLU
1	B	410	GLU
1	B	431	SER
1	B	435	LEU
1	B	438	ASN
1	B	447	ASN
1	B	449	GLU
1	B	450	LYS
1	B	454	LEU
1	B	476	GLU
1	B	478	SER
1	B	487	ARG
1	B	488	VAL
1	B	495	SER
1	B	511	SER
1	B	518	LYS

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Mol	Chain	Res	Type
1	B	548	LEU
1	B	558	LEU
1	B	571	LEU
1	B	610	LEU
1	B	617	LEU
1	B	619	LEU
1	B	629	THR
1	B	642	SER
1	B	645	MET
1	B	648	ASP
1	B	666	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	447	ASN
1	A	538	ASN
1	A	634	GLN
1	B	396	ASN
1	B	447	ASN

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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	1	2	24,33,33	2.50	7 (29%)	31,52,52	3.16	11 (35%)
4	ACY	A	7	-	1,3,3	3.17	1 (100%)	0,3,3	0.00	-
4	ACY	A	9	-	1,3,3	4.53	1 (100%)	0,3,3	0.00	-
3	ATP	B	2	2	24,33,33	2.71	8 (33%)	31,52,52	3.14	13 (41%)
4	ACY	B	8	-	1,3,3	1.46	0	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	ATP	A	1	2	-	0/18/38/38	0/3/3/3
4	ACY	A	7	-	-	0/0/0/0	0/0/0/0
4	ACY	A	9	-	-	0/0/0/0	0/0/0/0
3	ATP	B	2	2	-	0/18/38/38	0/3/3/3
4	ACY	B	8	-	-	0/0/0/0	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2	ATP	O5'-C5'	-4.92	1.24	1.44
3	A	1	ATP	O5'-C5'	-4.33	1.27	1.44
3	B	2	ATP	C8-N7	-2.49	1.29	1.34
3	B	2	ATP	PA-O5'	-2.41	1.48	1.59
3	A	1	ATP	PA-O5'	-2.17	1.49	1.59
3	A	1	ATP	C3'-C4'	-2.14	1.47	1.53
3	A	1	ATP	C2-N1	2.17	1.38	1.33
3	B	2	ATP	C2-N1	2.27	1.38	1.33
3	B	2	ATP	C2'-C3'	2.59	1.60	1.53
4	A	7	ACY	CH3-C	3.17	1.53	1.48
3	B	2	ATP	C2-N3	3.22	1.37	1.32
3	A	1	ATP	C2-N3	3.68	1.38	1.32
4	A	9	ACY	CH3-C	4.53	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ATP	O4'-C1'	6.32	1.49	1.41
3	A	1	ATP	C4-N3	6.59	1.45	1.35
3	B	2	ATP	C4-N3	6.91	1.45	1.35
3	B	2	ATP	O4'-C1'	7.28	1.50	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	ATP	O5'-PA-O1A	-7.20	81.68	109.62
3	B	2	ATP	O5'-PA-O1A	-6.66	83.75	109.62
3	A	1	ATP	C5'-C4'-C3'	-5.29	94.22	115.21
3	B	2	ATP	C5'-C4'-C3'	-5.18	94.66	115.21
3	B	2	ATP	PA-O3A-PB	-4.04	121.38	132.73
3	A	1	ATP	O4'-C4'-C5'	-3.25	97.70	109.32
3	B	2	ATP	N3-C2-N1	-3.08	126.53	128.89
3	B	2	ATP	O2A-PA-O5'	-2.73	94.71	108.46
3	A	1	ATP	O3A-PA-O5'	-2.71	95.76	102.94
3	A	1	ATP	N3-C2-N1	-2.48	126.99	128.89
3	A	1	ATP	PA-O3A-PB	-2.18	126.61	132.73
3	B	2	ATP	C1'-N9-C4	-2.15	123.70	126.94
3	B	2	ATP	O2A-PA-O1A	2.00	123.39	112.53
3	B	2	ATP	O3'-C3'-C2'	2.08	118.59	111.83
3	B	2	ATP	C4-C5-N7	2.14	111.45	109.48
3	A	1	ATP	C4-C5-N7	2.63	111.89	109.48
3	A	1	ATP	O2A-PA-O3A	2.92	118.32	105.09
3	B	2	ATP	O4'-C4'-C3'	3.01	111.20	105.15
3	B	2	ATP	O2A-PA-O3A	3.14	119.32	105.09
3	B	2	ATP	O2B-PB-O3B	3.34	120.25	105.09
3	A	1	ATP	O2B-PB-O3B	3.45	120.75	105.09
3	A	1	ATP	O4'-C4'-C3'	4.05	113.30	105.15
3	A	1	ATP	O5'-C5'-C4'	11.55	151.68	109.12
3	B	2	ATP	O5'-C5'-C4'	11.58	151.82	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7	ACY	2	0
3	B	2	ATP	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	264/286 (92%)	-0.25	0	100	100	54, 84, 111, 120	0
1	B	264/286 (92%)	-0.33	0	100	100	44, 78, 111, 120	0
All	All	528/572 (92%)	-0.29	0	100	100	44, 80, 111, 120	0

There are no RSRZ outliers to report.

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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	ACY	A	9	4/4	0.90	0.31	5.61	82,82,82,82	0
4	ACY	A	7	4/4	0.91	0.34	3.41	82,82,82,82	0
4	ACY	B	8	4/4	0.97	0.31	2.62	82,82,82,82	0
2	MG	B	4	1/1	0.97	0.21	1.96	82,82,82,82	0
3	ATP	A	1	31/31	0.88	0.23	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ATP	B	2	31/31	0.90	0.21	0.09	82,82,82,82	0
2	MG	A	3	1/1	0.96	0.13	-3.09	82,82,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.