Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:10 PM GMT

PDB ID	:	4XJX
Title	:	STRUCTURE OF MUTANT (E165H) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
Authors	:	Baikova, T.; Stsiapanava, A.; Moche, M.; Degtjarik, O.; Kuta-Smatanova, I.; Ettrich, R.
Deposited on	:	2015-01-09
Resolution	:	2.40 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
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

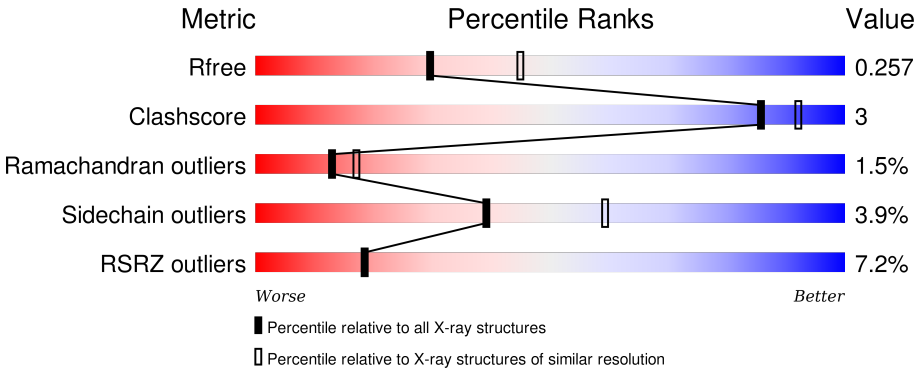
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	1038	6% 75% 7% • 17%
1	B	1038	6% 75% 7% • 17%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14686 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 HsdR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	1	0
			7062	4486	1195	1365	16			
1	B	863	Total	C	N	O	S	0	2	0
			7089	4502	1204	1367	16			

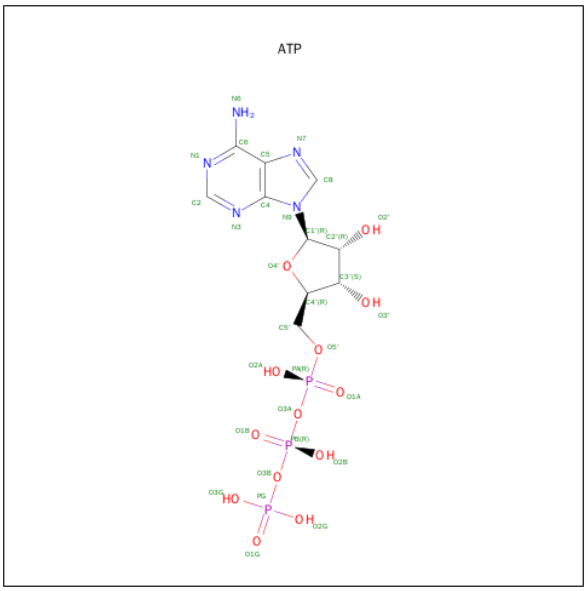
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	HIS	GLU	engineered mutation	UNP Q304R3
B	165	HIS	GLU	engineered mutation	UNP Q304R3

- 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: $C_{10}H_{16}N_5O_{13}P_3$).



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 water.

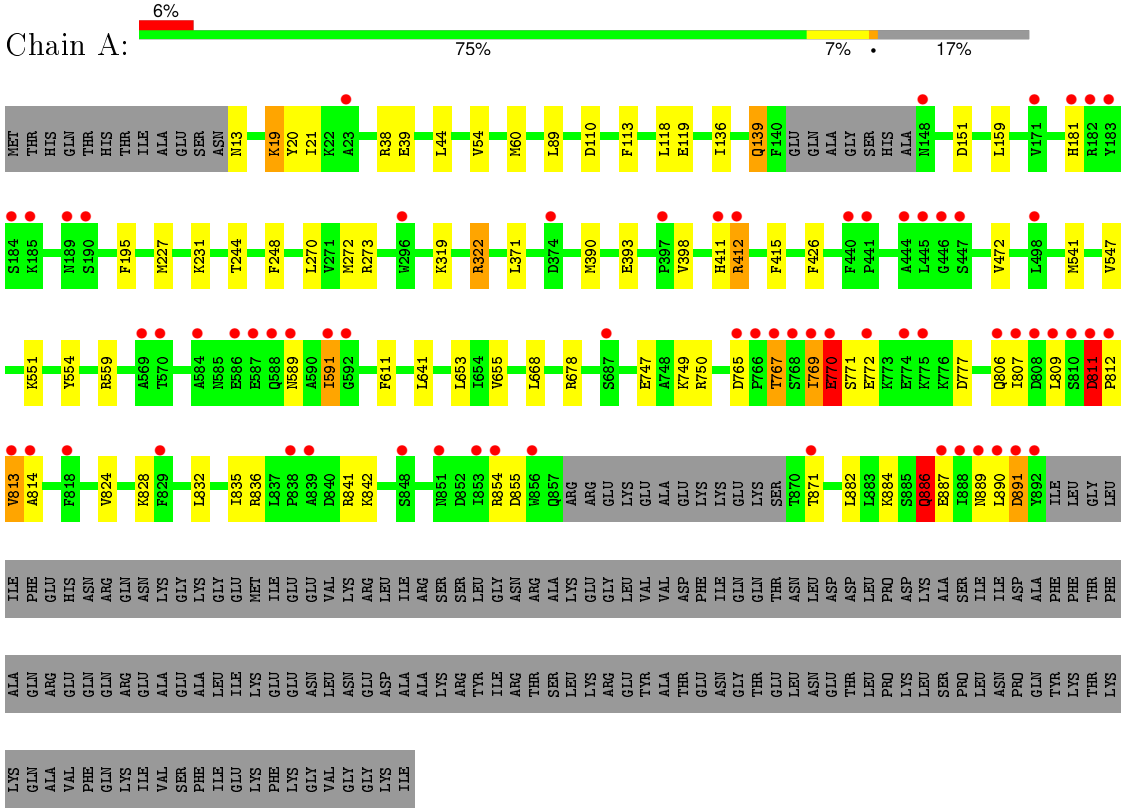
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	7
			220	220		
4	B	246	Total	O	0	5
			251	251		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

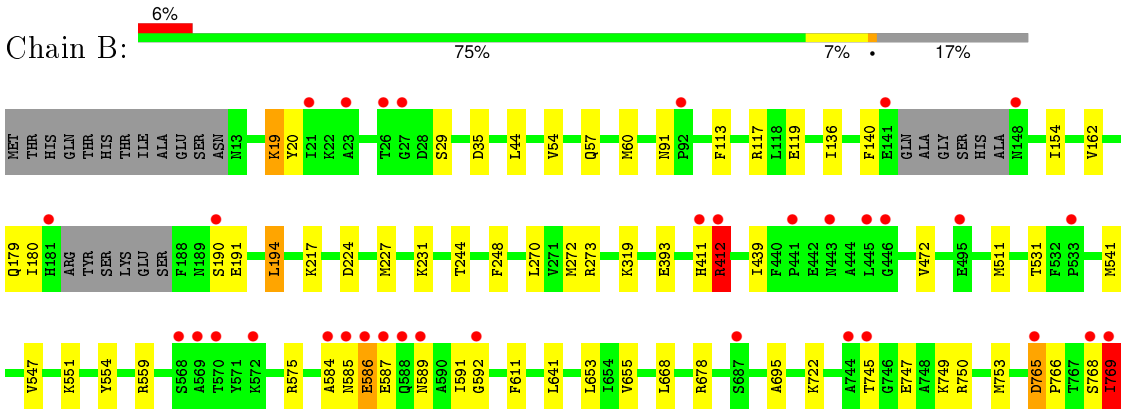
- Molecule 1: HsdR

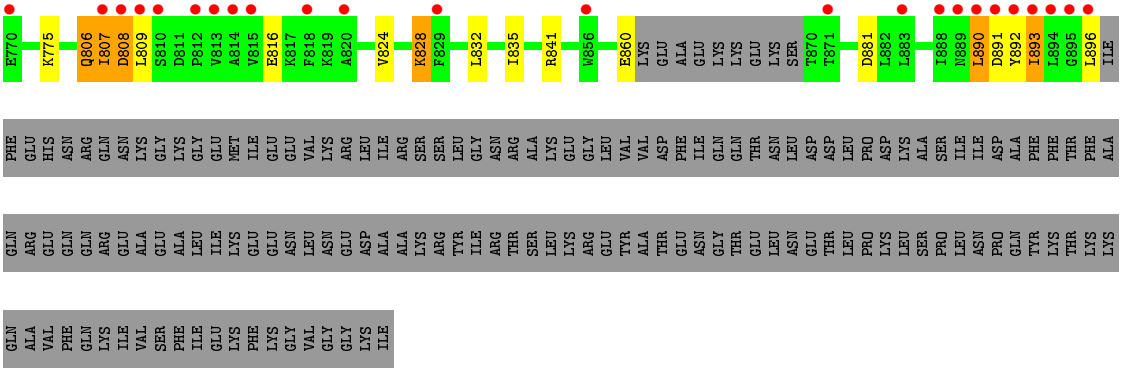
Chain A:



- Molecule 1: HsdR

Chain B:




E770 K775 Q806 I807 D808 L809 S810 D811 P812 V813 A814 V815 E816 K817 F818 K819 A820 V824 K828 F829 L832 I835 R841 W856 E860 T870 T871 D881 L882 L883 I888 N889 L890 D891 Y892 I893 L894 G895 L896 ILE
PHE GLU HIS ASN ARG GLN ASN LYS GLY LYS GLY GLU MET ILE GLU GLU VAL LYS ARG LEU ILE ARG SER SER LEU GLY ASN ARG ALA LYS GLU GLY LEU VAL VAL ASP PHE ILE GLN GLN THR ASN LEU ASP ASP LEU PRO ASP LYS ALA SER ILE ILE ASP ALA PHE PHE THR PHE ALA
GLN ARG GLU GLN GLN ARG GLU ALA GLU ALA LEU ILE LYS GLU GLU ASN LEU ASN GLU ASP ALA ALA LYS ARG TYR ILE ARG THR SER LEU LYS ARG GLU TYR ALA THR GLU ASN GLY THR GLU LEU ASN GLU THR LEU PRO LYS LEU SER PRO LEU ASN PRO GLN TYR LYS THR LYS LYS
GLN ALA VAL PHE GLN LYS ILE VAL SER PHE ILE GLU LYS PHE LYS GLY VAL GLY GLY LYS ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.22Å 124.54Å 128.54Å 90.00° 107.77° 90.00°	Depositor
Resolution (Å)	49.09 – 2.40 49.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.09-2.40) 99.3 (49.09-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.39Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.208 , 0.243 0.224 , 0.257	Depositor DCC
R_{free} test set	4976 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	38.1	Xtriage
Anisotropy	0.676	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.4	EDS
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 99539 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14686	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/7204	0.67	0/9719
1	B	0.50	0/7230	0.69	2/9753 (0.0%)
All	All	0.50	0/14434	0.68	2/19472 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	808	ASP	C-N-CA	6.58	138.16	121.70
1	B	806	GLN	C-N-CA	5.01	134.23	121.70

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	7062	0	6914	39	0
1	B	7089	0	6942	39	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	0	0
4	A	220	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	251	0	0	3	0
All	All	14686	0	13880	78	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 3.

All (78) 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:765:ASP:HB3	1:B:766:PRO:HD3	1.35	1.05
1:A:322:ARG:HG2	1:A:322:ARG:HH11	1.30	0.95
1:B:765:ASP:HB3	1:B:766:PRO:CD	2.03	0.88
1:B:54:VAL:HG11	1:B:60:MET:HG3	1.63	0.80
1:A:139:GLN:HG2	1:A:151:ASP:H	1.46	0.79
1:A:811:ASP:HB3	1:A:812:PRO:HD3	1.63	0.79
1:A:54:VAL:HG11	1:A:60:MET:HG3	1.65	0.78
1:A:811:ASP:HB3	1:A:812:PRO:CD	2.13	0.78
1:A:272:MET:CE	1:A:319:LYS:HG2	2.24	0.68
1:B:559:ARG:HD2	4:B:1249:HOH:O	1.94	0.68
1:B:765:ASP:CB	1:B:766:PRO:HD3	2.21	0.67
1:B:272:MET:CE	1:B:319:LYS:HG2	2.23	0.67
1:A:809:LEU:HB2	1:A:813:VAL:HG11	1.79	0.63
1:B:54:VAL:HG11	1:B:60:MET:CG	2.29	0.63
1:A:813:VAL:HG22	1:A:814:ALA:H	1.64	0.62
1:A:591:ILE:HG12	1:A:678:ARG:HG3	1.79	0.62
1:B:272:MET:HE1	1:B:319:LYS:HG2	1.80	0.62
1:A:541:MET:HG3	1:A:668:LEU:HD11	1.83	0.60
1:A:227:MET:HE3	1:A:273:ARG:HG3	1.84	0.59
1:A:322:ARG:CG	1:A:322:ARG:HH11	2.10	0.58
1:A:272:MET:HE1	1:A:319:LYS:HG2	1.84	0.58
1:B:227:MET:HE3	1:B:273:ARG:HG3	1.86	0.58
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.85	0.58
1:B:586:GLU:HG2	1:B:589:ASN:HA	1.86	0.57
1:B:57:GLN:HG3	1:B:194:LEU:HD22	1.86	0.57
1:B:592:GLY:HA2	1:B:678:ARG:HB2	1.87	0.56
1:A:272:MET:HE2	1:A:319:LYS:HG2	1.89	0.55
1:A:554:TYR:HB3	1:A:611:PHE:HZ	1.73	0.54
1:A:811:ASP:CB	1:A:812:PRO:HD3	2.37	0.54
1:A:824:VAL:HG13	1:A:828:LYS:HB3	1.90	0.54
1:A:113:PHE:HE1	1:A:119:GLU:HB2	1.74	0.53
1:B:272:MET:HE2	1:B:319:LYS:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:TYR:HB3	1:B:611:PHE:HZ	1.74	0.52
1:A:412:ARG:HA	1:A:415:PHE:HB3	1.93	0.50
1:B:113:PHE:HE1	1:B:119:GLU:HB2	1.76	0.50
1:B:753:MET:HA	1:B:753:MET:CE	2.41	0.50
1:A:19:LYS:HE3	1:A:20:TYR:H	1.77	0.50
1:B:824:VAL:HG13	1:B:828:LYS:HB3	1.93	0.50
1:A:809:LEU:HB2	1:A:813:VAL:CG1	2.42	0.49
1:B:91:ASN:HB3	4:B:1269:HOH:O	2.13	0.49
1:B:19:LYS:HE3	1:B:20:TYR:H	1.77	0.49
1:B:745:THR:OG1	1:B:747:GLU:HG2	2.13	0.49
1:B:641:LEU:HD11	1:B:653:LEU:HD13	1.95	0.49
1:B:765:ASP:CB	1:B:766:PRO:CD	2.87	0.48
1:A:641:LEU:HD11	1:A:653:LEU:HD13	1.95	0.47
1:A:770:GLU:HB3	1:A:771:SER:H	1.52	0.47
1:A:769:ILE:HG23	1:A:770:GLU:H	1.80	0.47
1:B:244:THR:HA	1:B:248:PHE:HB2	1.98	0.45
1:A:559:ARG:HD2	4:A:1237:HOH:O	2.17	0.45
1:A:244:THR:HA	1:A:248:PHE:HB2	1.99	0.45
1:A:390:MET:HE1	1:A:426:PHE:CE2	2.52	0.45
1:A:227:MET:CE	1:A:273:ARG:HG3	2.45	0.45
1:B:227:MET:CE	1:B:273:ARG:HG3	2.46	0.44
1:A:547:VAL:O	1:A:551:LYS:HG3	2.17	0.44
1:B:893:ILE:HG13	1:B:893:ILE:H	1.70	0.44
1:A:21:ILE:HG13	1:A:21:ILE:O	2.18	0.44
1:B:695:ALA:HB3	1:B:881:ASP:HB2	2.00	0.44
1:B:412:ARG:H	1:B:412:ARG:HD2	1.82	0.44
1:B:769:ILE:HG22	1:B:775:LYS:HG2	2.00	0.43
1:A:44:LEU:HD13	1:A:136:ILE:HG21	1.99	0.43
1:B:412:ARG:HD3	1:B:439:ILE:HD11	2.00	0.43
1:B:44:LEU:HD13	1:B:136:ILE:HG21	2.00	0.43
1:A:886:GLN:HB2	1:A:887:GLU:H	1.60	0.43
1:B:231:LYS:HE2	4:B:1414:HOH:O	2.18	0.43
1:A:110:ASP:HB3	1:A:118:LEU:HD11	2.01	0.43
1:B:807:ILE:HG23	1:B:808:ASP:N	2.34	0.42
1:B:29:SER:O	1:B:35:ASP:HB3	2.19	0.42
1:B:591:ILE:HG22	1:B:678:ARG:CG	2.49	0.42
1:A:60:MET:HE1	1:A:195:PHE:HE2	1.85	0.41
1:A:832:LEU:HA	1:A:835:ILE:HD12	2.02	0.41
1:B:832:LEU:HA	1:B:835:ILE:HD12	2.02	0.41
1:A:20:TYR:HB3	1:A:231[A]:LYS:HD3	2.02	0.41
1:B:154:ILE:HB	1:B:162:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:LEU:C	1:B:892:TYR:H	2.23	0.41
1:A:371:LEU:HD22	1:A:398:VAL:HG21	2.02	0.41
1:B:547:VAL:O	1:B:551:LYS:HG3	2.21	0.41
1:A:322:ARG:HG2	1:A:322:ARG:NH1	2.11	0.40
1:A:89:LEU:HD11	1:A:159:LEU:HD21	2.03	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	856/1038 (82%)	790 (92%)	51 (6%)	15 (2%)	11	13
1	B	857/1038 (83%)	792 (92%)	54 (6%)	11 (1%)	15	21
All	All	1713/2076 (82%)	1582 (92%)	105 (6%)	26 (2%)	13	17

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	HIS
1	A	767	THR
1	A	770	GLU
1	A	811	ASP
1	A	886	GLN
1	A	891	ASP
1	B	411	HIS
1	B	585	ASN
1	B	765	ASP
1	B	807	ILE
1	A	591	ILE
1	A	813	VAL
1	A	889	ASN

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Mol	Chain	Res	Type
1	B	140	PHE
1	B	190	SER
1	B	768	SER
1	A	769	ILE
1	A	871	THR
1	A	884	LYS
1	B	412	ARG
1	B	584	ALA
1	B	769	ILE
1	B	891	ASP
1	A	412	ARG
1	A	589	ASN
1	A	855	ASP

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	775/927 (84%)	745 (96%)	30 (4%)	39	59
1	B	777/927 (84%)	746 (96%)	31 (4%)	38	58
All	All	1552/1854 (84%)	1491 (96%)	61 (4%)	39	59

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	19	LYS
1	A	38	ARG
1	A	39	GLU
1	A	139	GLN
1	A	181	HIS
1	A	270	LEU
1	A	322	ARG
1	A	393	GLU
1	A	472	VAL

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Mol	Chain	Res	Type
1	A	655	VAL
1	A	747	GLU
1	A	749	LYS
1	A	750	ARG
1	A	765	ASP
1	A	767	THR
1	A	770	GLU
1	A	772	GLU
1	A	777	ASP
1	A	806	GLN
1	A	807	ILE
1	A	811	ASP
1	A	836	ARG
1	A	841	ARG
1	A	842	LYS
1	A	854	ARG
1	A	882	LEU
1	A	886	GLN
1	A	890	LEU
1	A	891	ASP
1	B	19	LYS
1	B	117	ARG
1	B	179	GLN
1	B	180	ILE
1	B	191	GLU
1	B	194	LEU
1	B	217	LYS
1	B	224	ASP
1	B	270	LEU
1	B	393	GLU
1	B	412	ARG
1	B	472	VAL
1	B	511	MET
1	B	531	THR
1	B	575	ARG
1	B	586	GLU
1	B	587	GLU
1	B	655	VAL
1	B	722	LYS
1	B	749	LYS
1	B	750	ARG
1	B	769	ILE

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Mol	Chain	Res	Type
1	B	806	GLN
1	B	809	LEU
1	B	816	GLU
1	B	828	LYS
1	B	841	ARG
1	B	860	GLU
1	B	890	LEU
1	B	893	ILE
1	B	896	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	1102	2	26,33,33	0.68	0	26,52,52	0.85	1 (3%)
3	ATP	B	1102	2	26,33,33	0.72	0	26,52,52	0.85	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	1102	2	-	0/18/38/38	0/3/3/3
3	ATP	B	1102	2	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1102	ATP	O3G-PG-O2G	2.61	117.02	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	861/1038 (82%)	0.33	66 (7%)	16 16	29, 50, 102, 134	0
1	B	863/1038 (83%)	0.17	58 (6%)	21 21	25, 46, 95, 129	0
All	All	1724/2076 (83%)	0.25	124 (7%)	18 18	25, 48, 99, 134	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	810	SER	15.9
1	A	445	LEU	11.5
1	A	813	VAL	10.5
1	A	811	ASP	8.1
1	A	766	PRO	7.9
1	A	183	TYR	7.7
1	A	888	ILE	7.3
1	B	896	LEU	7.2
1	B	813	VAL	7.2
1	A	812	PRO	6.7
1	A	592	GLY	6.4
1	B	768	SER	6.4
1	A	446	GLY	6.3
1	A	767	THR	6.0
1	B	809	LEU	5.8
1	B	890	LEU	5.8
1	B	587	GLU	5.2
1	B	589	ASN	5.2
1	A	856	TRP	5.1
1	A	182	ARG	5.1
1	A	588	GLN	5.1
1	B	894	LEU	5.1
1	B	810	SER	4.9
1	A	412	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	588	GLN	4.9
1	B	592	GLY	4.7
1	A	441	PRO	4.6
1	A	814	ALA	4.6
1	A	829	PHE	4.4
1	B	892	TYR	4.4
1	A	892	TYR	4.3
1	A	807	ILE	4.2
1	B	893	ILE	4.2
1	B	812	PRO	4.1
1	B	181	HIS	4.1
1	B	570	THR	4.1
1	B	814	ALA	4.1
1	A	809	LEU	4.0
1	A	854	ARG	4.0
1	B	586	GLU	4.0
1	A	444	ALA	3.9
1	A	808	ASP	3.9
1	A	570	THR	3.8
1	A	591	ILE	3.8
1	A	818	PHE	3.8
1	A	587	GLU	3.8
1	A	190	SER	3.8
1	B	141	GLU	3.7
1	B	769	ILE	3.7
1	A	890	LEU	3.6
1	B	446	GLY	3.6
1	A	851	ASN	3.5
1	B	815	VAL	3.5
1	A	887	GLU	3.4
1	B	891	ASP	3.4
1	B	889	ASN	3.4
1	A	768	SER	3.4
1	A	148	ASN	3.4
1	B	871	THR	3.4
1	A	848	SER	3.3
1	B	818	PHE	3.3
1	A	769	ILE	3.3
1	B	856	TRP	3.3
1	B	585	ASN	3.2
1	A	889	ASN	3.2
1	B	807	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	189	ASN	3.1
1	A	184	SER	3.1
1	B	584	ALA	3.1
1	B	770	GLU	3.1
1	A	498	LEU	3.1
1	A	871	THR	3.1
1	B	829	PHE	3.0
1	A	584	ALA	3.0
1	A	569	ALA	3.0
1	B	23	ALA	2.9
1	B	411	HIS	2.9
1	B	21	ILE	2.9
1	A	891	ASP	2.8
1	A	185	LYS	2.8
1	B	820	ALA	2.8
1	B	412	ARG	2.8
1	A	586	GLU	2.8
1	A	770	GLU	2.8
1	A	774	GLU	2.7
1	B	441	PRO	2.7
1	A	589	ASN	2.7
1	B	744	ALA	2.7
1	B	687	SER	2.6
1	B	495	GLU	2.6
1	A	296	TRP	2.6
1	B	765	ASP	2.6
1	B	26	THR	2.6
1	A	838	PRO	2.5
1	A	411	HIS	2.5
1	A	440	PHE	2.5
1	A	853	ILE	2.5
1	B	568	SER	2.5
1	B	745	THR	2.4
1	A	772	GLU	2.4
1	B	445	LEU	2.4
1	B	27	GLY	2.4
1	B	569	ALA	2.3
1	B	895	GLY	2.3
1	A	839	ALA	2.2
1	B	888	ILE	2.2
1	B	190	SER	2.2
1	A	181	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	148	ASN	2.2
1	A	806	GLN	2.2
1	A	374	ASP	2.1
1	B	533	PRO	2.1
1	A	447	SER	2.1
1	A	687	SER	2.1
1	A	23	ALA	2.1
1	A	765	ASP	2.1
1	B	572	LYS	2.1
1	B	883	LEU	2.1
1	B	92	PRO	2.0
1	B	808	ASP	2.0
1	A	171	VAL	2.0
1	A	397	PRO	2.0
1	A	775	LYS	2.0
1	B	443	ASN	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^{th} 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
3	ATP	A	1102	31/31	0.98	0.18	-0.41	26,35,40,41	0
3	ATP	B	1102	31/31	0.98	0.18	-0.71	25,33,38,38	0
2	MG	B	1101	1/1	0.97	0.17	-	33,33,33,33	0
2	MG	A	1101	1/1	0.97	0.15	-	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.