



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:57 am GMT

PDB ID : 4BEB
Title : MUTANT (K220E) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP
Authors : Csefalvay, E.; Lapkouski, M.; Guzanova, A.; Csefalvay, L.; Baikova, T.; Shevelev, I.; Janscak, P.; Smatanova, I.K.; Panjekar, S.; Carey, J.; Weiserova, M.; Ettrich, R.
Deposited on : 2013-03-07
Resolution : 2.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

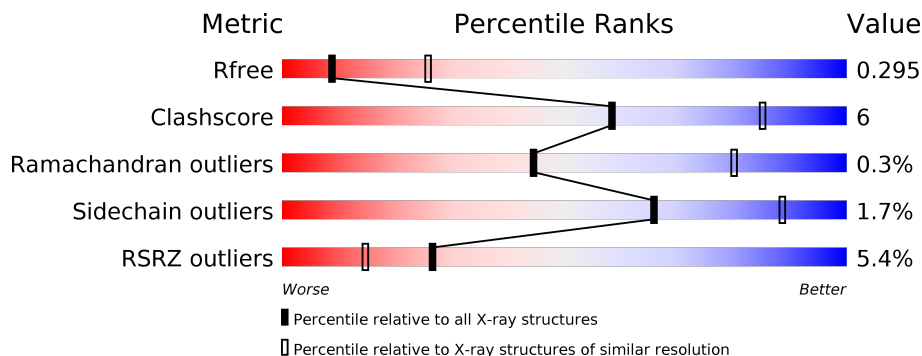
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2168 (3.00-2.96)
Clashscore	112137	2535 (3.00-2.96)
Ramachandran outliers	110173	2451 (3.00-2.96)
Sidechain outliers	110143	2454 (3.00-2.96)
RSRZ outliers	101464	2192 (3.00-2.96)

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 $\leq 5\%$. 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	1038	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	1038	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	1038	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>10%</div> <div>•</div> <div>19%</div> </div> </div>
1	D	1038	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>12%</div> <div>•</div> <div>20%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27369 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 TYPE I RESTRICTION ENZYME HSDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	839	Total	C	N	O	S	0	0	0
			6821	4340	1158	1307	16			
1	B	842	Total	C	N	O	S	0	0	0
			6846	4353	1158	1319	16			
1	C	838	Total	C	N	O	S	0	0	0
			6802	4326	1151	1309	16			
1	D	833	Total	C	N	O	S	0	0	0
			6772	4309	1146	1301	16			

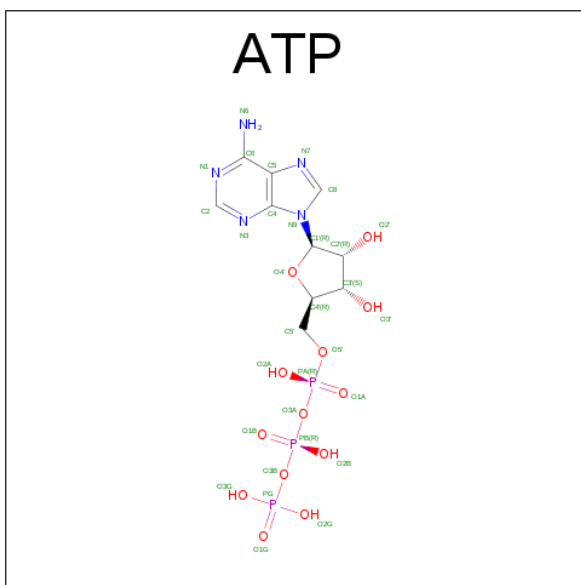
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
B	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
C	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3
D	220	GLU	LYS	ENGINEERED MUTATION	UNP Q304R3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

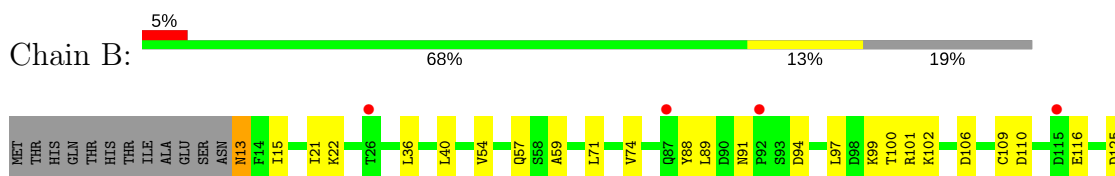
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

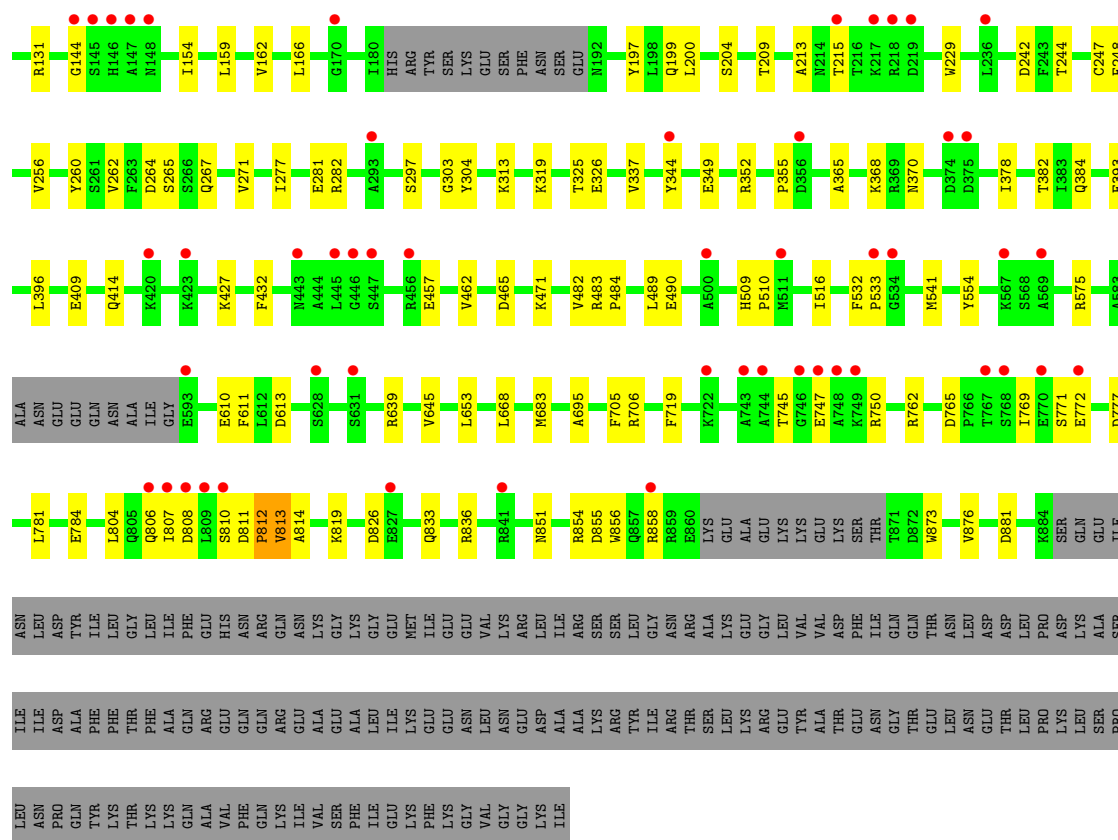
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



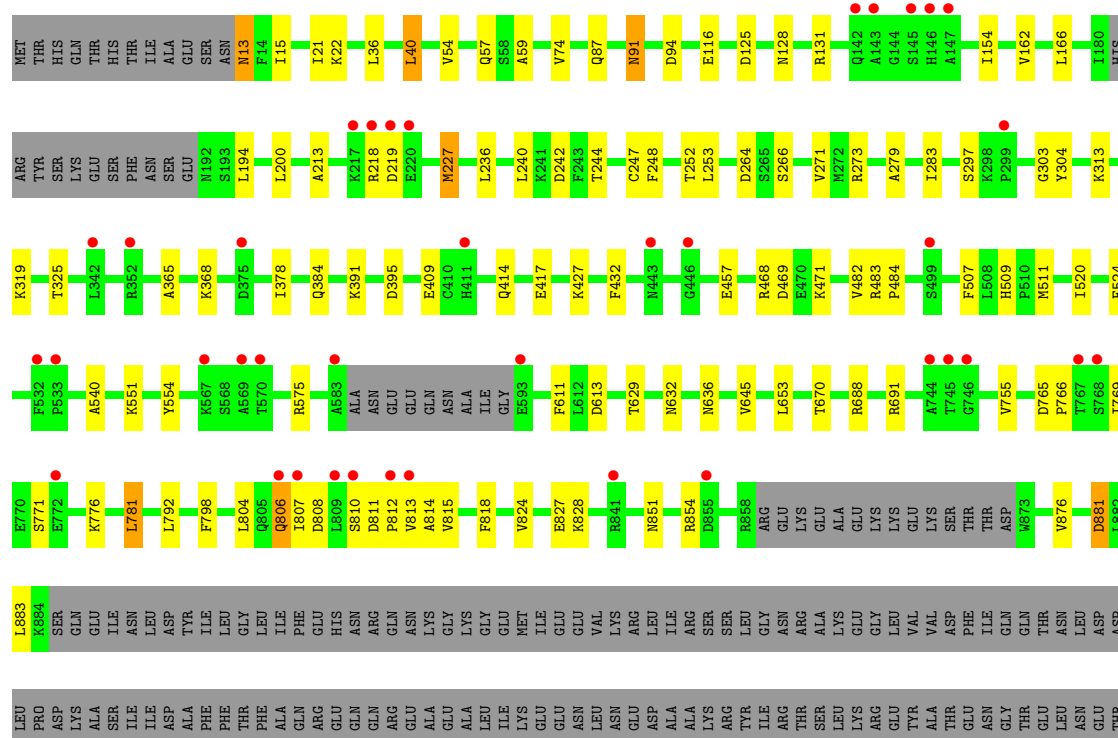
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	C	1	Total 31	C 10	N 5	O 13	P 3	0	0
3	D	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 1: TYPE I RESTRICTION ENZYME HSDR





• Molecule 1: TYPE I RESTRICTION ENZYME HSDR



LEU	PRO	THR	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	LYS	ILE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 1: TYPE I RESTRICTION ENZYME HSDR



VAL	PHE	GLN	GLN	GLN	GLN	VAL	SER	PHE	ILE	GLU	ILE	GLU	GLU	GLU	GLU	ASN	ASN	GLU	GLU	GLU	GLU	GLU	THR	SER	ALA	THR	THR	GLU	GLY	GLN	THR	THR	GLU	LEU	ASN	ASN	ASP	GLN	TYR	PHE	THR	THR	LYS	LYS	ALA	ALA						
GLN	GLN	GLN	GLN	GLN	GLN	VAL	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY						
THR	HIS	THR	HIS	THR	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR						
R149	I154	L159	V162	Q163	I164	E165	L166	V171	Q179	I180	HIS	ARG	TYR	SER	LYS	GLU	SER	PHE	ASN	SER	N192	S193	L194	Y197	S204	N205	G206	T209	A213	N214	T215	T216	K217	R218	D219	S232	L236	D239	L240	V256	Y260	S261	V262	F263								
D264	S265	V271	L277	T280	T292	S297	K298	P299	E300	G303	Y304	K313	T314	L315	L323	F334	K340	S344	M347	K348	E349	Y350	Q351	R352	D356	A365	K368	L371	D375	Q384	K391	Q402	E409	Q414	E417																	
K427	Y430	Q431	F432	E442	E457	V462	D465	R468	K471	V482	R483	T483	K496	F507	L508	H509	P510	M511	T531	F532	P533	G534	S535	K536	M541	Y541	Y554	E562	T570	Y571	R575	S581	F582	A583	ALA	ASN	GLU	GLN	ASN	ILE												
GLY	E593	M604	F611	R617	K624	S631	M632	G633	F634	R639	L668	M683	F719	K722	N723	T741	A744	T745	G746	E747	A748	M753	T754	V755	D765	P766	T767	S768	I769	E770	E772	K775	L781	L792	F798	L804	Q805	P806	ALA	ALA	ARG											
D808	L809	S810	D811	V812	V813	A814	K817	F818	K819	H822	D826	E827	K828	R836	D840	R841	D855	R858	R859	GLU	LYS	GLU	ALA	GLU	VAL	VAL	ASP	PHE	GLU	GLY	GLN	THR	T871	D872	W873	V876	K884	SER	GLN	GLU	ILE	ASN	LEU	ASP	TYR	ILE	PHE	THR	PHE	ALA	GLN	ALA
HIS	ASN	ARG	GLN	ASN	LYS	GLY	GLY	GLU	MET	ILE	GLU	GLU	VAL	ASN	LEU	ASN	GLU	ARG	ILE	ARG	SER	SER	GLY	THR	ALA	LYS	THR	THR	GLY	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
GLU	GLN	ARG	GLU	ASN	LYS	GLY	GLY	GLU	GLY	GLY	GLY	GLY	VAL	ASN	LEU	ASN	GLU	ARG	ILE	ARG	SER	SER	GLY	THR	ALA	LYS	THR	THR	GLY	GLN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR				
PHE	GLN	LYS	ILE	VAL	SER	PHE	ILE	GLU	LYS	PHE	GLY	VAL	GLY	LYS	GLY	LYS	ILE	THR	ARG	ARG	THR	SER	LEU	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR			
THR	HIS	THR	HIS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	127.11Å 123.11Å 160.11Å 90.00° 111.48° 90.00°	Depositor
Resolution (Å)	19.89 – 2.99 19.88 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.89-2.99) 98.4 (19.88-2.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.98Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.255 , 0.296 0.254 , 0.295	Depositor DCC
R_{free} test set	966 reflections (1.06%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	1.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	27369	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2132e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.27	0/6954	0.51	1/9383 (0.0%)
1	B	0.25	0/6979	0.50	1/9418 (0.0%)
1	C	0.27	0/6933	0.49	0/9355
1	D	0.25	0/6901	0.48	1/9309 (0.0%)
All	All	0.26	0/27767	0.50	3/37465 (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	A	0	4
1	B	0	4
1	C	0	2
1	D	0	3
All	All	0	13

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	813	VAL	N-CA-C	7.00	129.89	111.00
1	B	813	VAL	N-CA-C	6.66	128.98	111.00
1	D	534	GLY	N-CA-C	5.49	126.81	113.10

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	ALA	Peptide
1	A	769	ILE	Peptide
1	A	806	GLN	Peptide
1	A	812	PRO	Peptide
1	B	144	GLY	Peptide

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	6821	0	6660	83	0
1	B	6846	0	6672	78	0
1	C	6802	0	6636	67	0
1	D	6772	0	6607	75	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0
All	All	27369	0	26623	297	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 6.

The worst 5 of 297 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ALA:HB1	1:A:148:ASN:HA	1.49	0.93
1:A:807:ILE:H	1:A:808:ASP:HB2	1.39	0.86
1:B:807:ILE:H	1:B:808:ASP:HB2	1.44	0.81
1:C:807:ILE:H	1:C:808:ASP:HB2	1.46	0.80
1:D:859:ARG:H	1:D:859:ARG:HH11	1.27	0.79

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	831/1038 (80%)	793 (95%)	36 (4%)	2 (0%)	51	85
1	B	834/1038 (80%)	800 (96%)	32 (4%)	2 (0%)	51	85
1	C	830/1038 (80%)	796 (96%)	33 (4%)	1 (0%)	55	88
1	D	821/1038 (79%)	782 (95%)	35 (4%)	4 (0%)	32	72
All	All	3316/4152 (80%)	3171 (96%)	136 (4%)	9 (0%)	44	80

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	746	GLY
1	D	813	VAL
1	A	765	ASP
1	C	813	VAL
1	B	813	VAL

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	737/927 (80%)	724 (98%)	13 (2%)	64	88
1	B	741/927 (80%)	727 (98%)	14 (2%)	62	87
1	C	736/927 (79%)	722 (98%)	14 (2%)	62	87
1	D	733/927 (79%)	725 (99%)	8 (1%)	78	93
All	All	2947/3708 (80%)	2898 (98%)	49 (2%)	66	88

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	610	GLU
1	C	13	ASN
1	D	753	MET
1	B	771	SER
1	C	21	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	GLN
1	D	57	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 8 ligands modelled in this entry, 4 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	ATP	A	1886	2	27,33,33	0.95	1 (3%)	25,52,52	1.64	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ATP	B	1886	2	27,33,33	0.99	1 (3%)	25,52,52	1.61	2 (8%)
3	ATP	C	1886	2	27,33,33	0.93	1 (3%)	25,52,52	1.64	2 (8%)
3	ATP	D	1886	2	27,33,33	0.97	1 (3%)	25,52,52	1.63	2 (8%)

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	1886	2	-	0/18/38/38	0/3/3/3
3	ATP	B	1886	2	-	0/18/38/38	0/3/3/3
3	ATP	C	1886	2	-	0/18/38/38	0/3/3/3
3	ATP	D	1886	2	-	0/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1886	ATP	C5-C4	3.00	1.47	1.40
3	A	1886	ATP	C5-C4	3.04	1.47	1.40
3	D	1886	ATP	C5-C4	3.12	1.47	1.40
3	B	1886	ATP	C5-C4	3.17	1.47	1.40

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1886	ATP	N3-C2-N1	-5.98	123.65	128.86
3	B	1886	ATP	N3-C2-N1	-5.81	123.79	128.86
3	D	1886	ATP	N3-C2-N1	-5.78	123.83	128.86
3	C	1886	ATP	N3-C2-N1	-5.77	123.83	128.86
3	B	1886	ATP	C4-C5-N7	-3.00	106.51	109.41

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	C	1886	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	839/1038 (80%)	0.01	40 (4%)	31	18	20, 42, 79, 109	0
1	B	842/1038 (81%)	0.26	55 (6%)	20	10	38, 58, 86, 115	0
1	C	838/1038 (80%)	0.01	38 (4%)	34	19	21, 42, 79, 105	0
1	D	833/1038 (80%)	0.33	48 (5%)	24	13	41, 62, 91, 117	0
All	All	3352/4152 (80%)	0.15	181 (5%)	26	15	20, 54, 85, 117	0

The worst 5 of 181 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	767	THR	10.0
1	C	145	SER	8.4
1	A	767	THR	8.1
1	D	583	ALA	6.2
1	C	767	THR	6.2

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(\AA^2)	Q<0.9
3	ATP	D	1886	31/31	0.95	0.14	-1.05	45,51,60,62	0
3	ATP	C	1886	31/31	0.97	0.13	-1.05	21,29,39,40	0
3	ATP	A	1886	31/31	0.97	0.12	-1.33	27,34,43,51	0
3	ATP	B	1886	31/31	0.96	0.12	-1.57	42,50,57,61	0
2	MG	C	1885	1/1	0.91	0.15	-	37,37,37,37	0
2	MG	A	1885	1/1	0.92	0.20	-	45,45,45,45	0
2	MG	B	1885	1/1	0.80	0.21	-	52,52,52,52	0
2	MG	D	1885	1/1	0.88	0.27	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.