



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:59 am GMT

PDB ID : 4BE7  
Title : MUTANT (K220R) OF THE HSDR SUBUNIT OF THE ECOR124I RESTRICTION ENZYME IN COMPLEX WITH ATP  
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Deposited on : 2013-03-06  
Resolution : 2.74 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (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

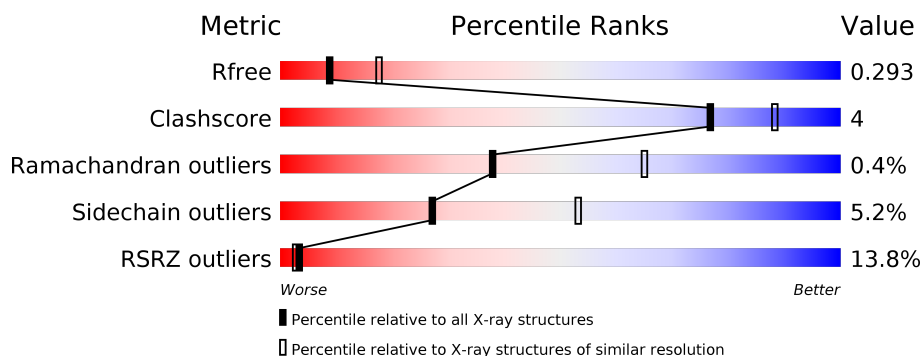
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3342 (2.78-2.70)
Clashscore	112137	3731 (2.78-2.70)
Ramachandran outliers	110173	3670 (2.78-2.70)
Sidechain outliers	110143	3671 (2.78-2.70)
RSRZ outliers	101464	3362 (2.78-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1038	<div> <div>9%</div> <div>71%</div> <div>8%</div> <div>19%</div> </div>
1	D	1038	<div> <div>13%</div> <div>70%</div> <div>9%</div> <div>20%</div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13387 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.

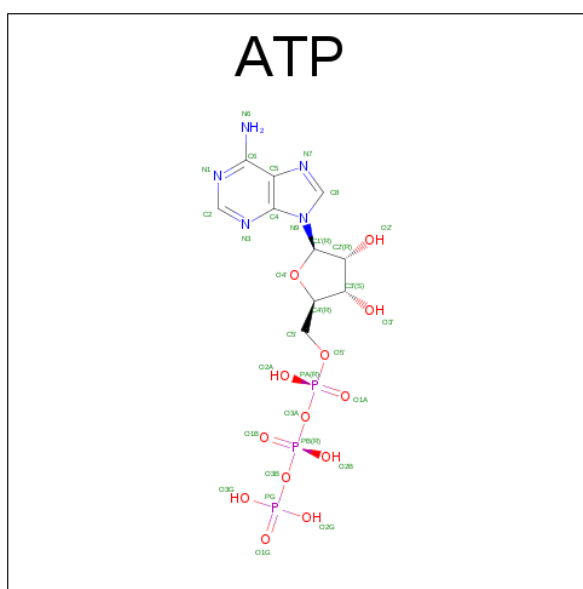
- Molecule 1 is a protein called TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	837	Total	C	N	O	S	0	0	0
			6631	4226	1112	1277	16			
1	D	835	Total	C	N	O	S	0	0	0
			6594	4204	1106	1268	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	220	ARG	LYS	ENGINEERED MUTATION	UNP Q304R3
D	220	ARG	LYS	ENGINEERED MUTATION	UNP Q304R3

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



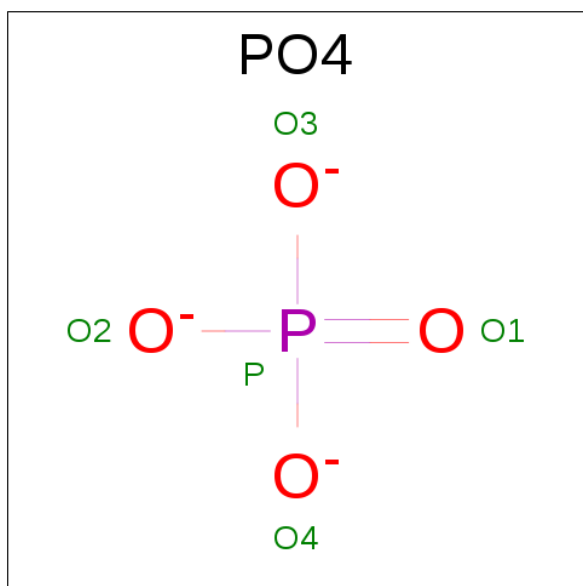
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

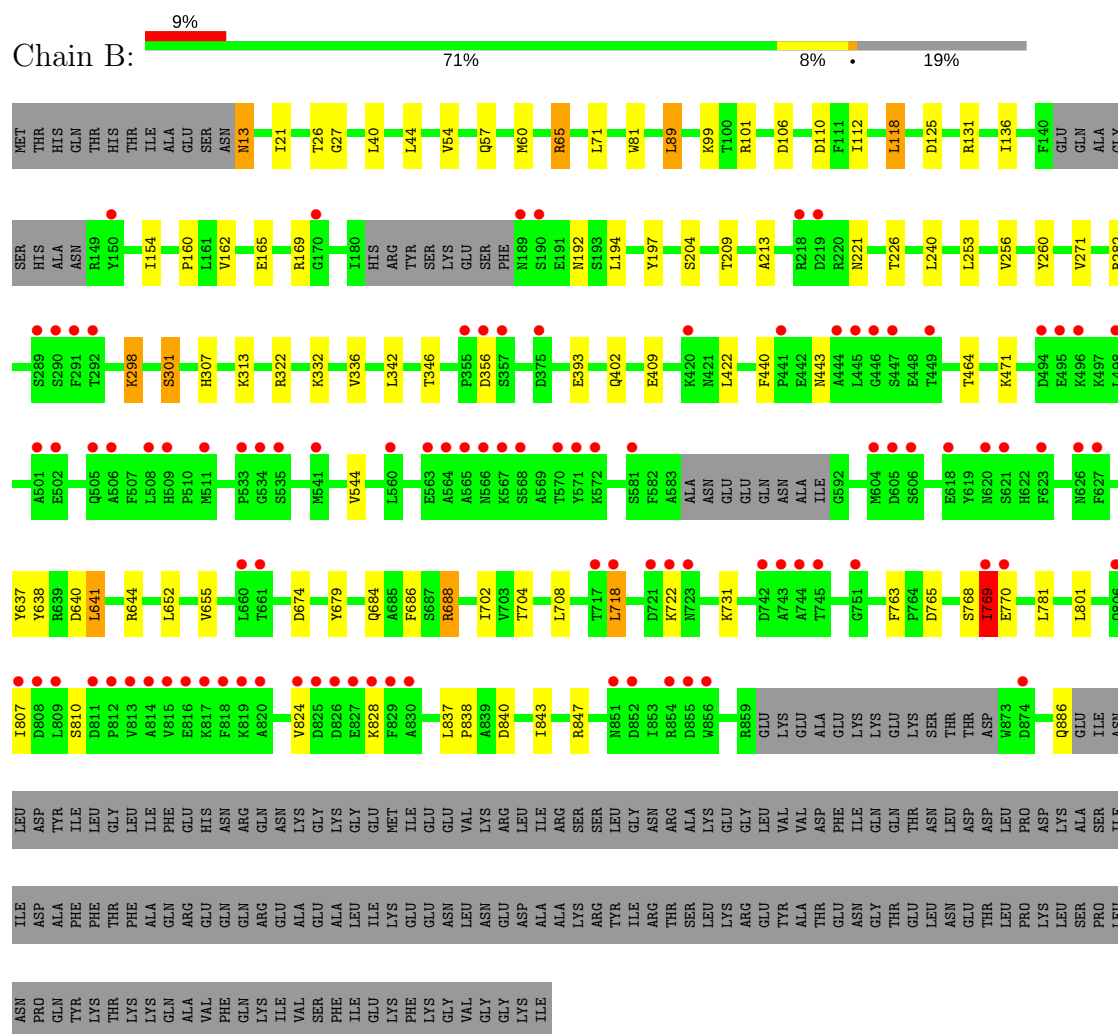
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	45	Total 45	O 45	0	0
5	D	33	Total 33	O 33	0	0

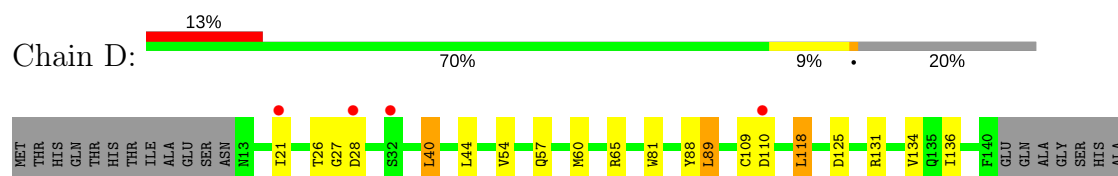
### 3 Residue-property plots [i](#)

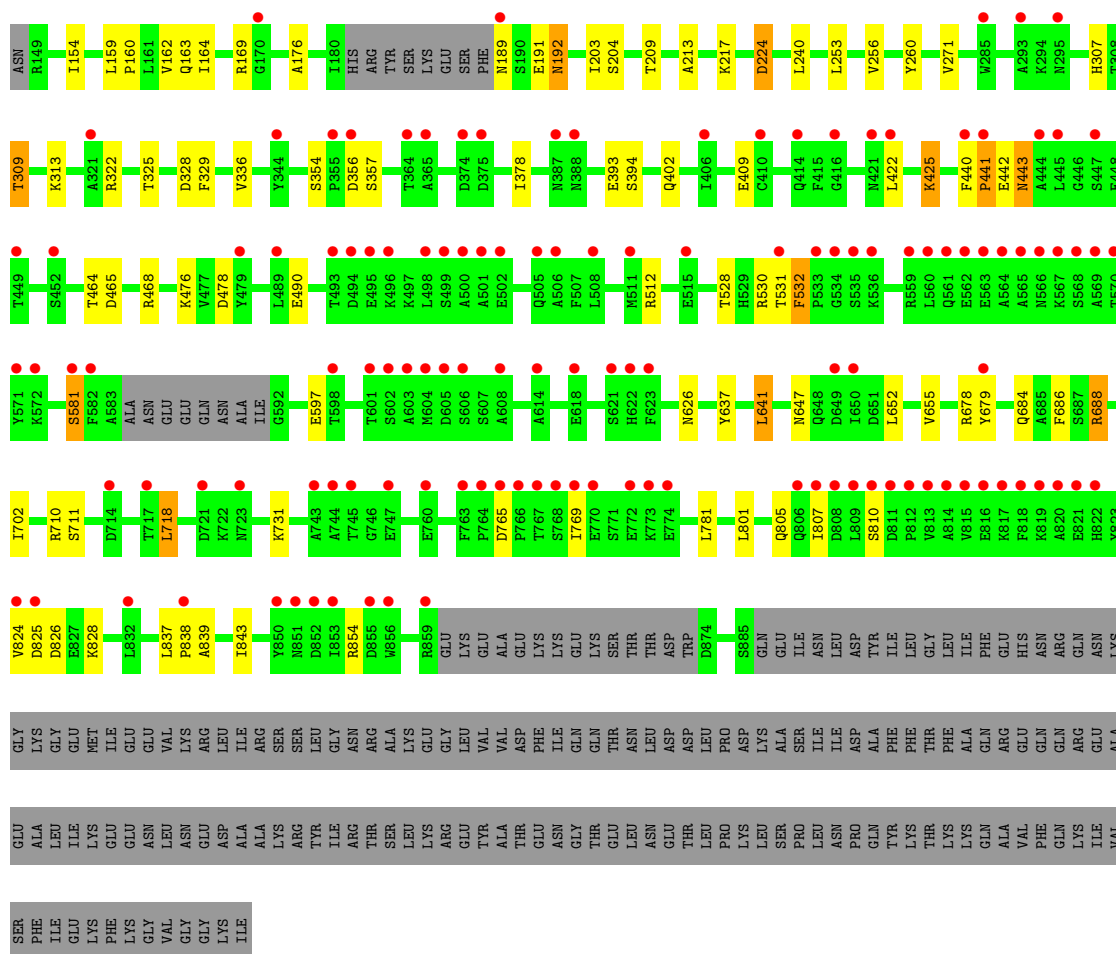
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN



#### • Molecule 1: TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.05Å 124.35Å 128.01Å 90.00° 108.86° 90.00°	Depositor
Resolution (Å)	32.36 – 2.74 33.73 – 2.74	Depositor EDS
% Data completeness (in resolution range)	93.2 (32.36-2.74) 93.5 (33.73-2.74)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.249 , 0.292 0.249 , 0.293	Depositor DCC
$R_{free}$ test set	3192 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	13387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, PO4, 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	B	0.27	0/6760	0.52	1/9146 (0.0%)
1	D	0.27	0/6721	0.53	3/9097 (0.0%)
All	All	0.27	0/13481	0.53	4/18243 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	441	PRO	C-N-CA	6.15	137.08	121.70
1	D	441	PRO	CA-C-N	5.29	128.83	117.20
1	B	769	ILE	N-CA-C	-5.26	96.79	111.00
1	D	826	ASP	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

There are no planarity outliers.

### 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	B	6631	0	6305	44	0
1	D	6594	0	6268	47	0
2	B	31	0	12	1	0
2	D	31	0	12	1	0
3	B	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	45	0	0	1	0
5	D	33	0	0	1	0
All	All	13387	0	12597	91	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 4.

All (91) 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:D:824:VAL:HG13	1:D:828:LYS:HB3	1.54	0.90
1:D:27:GLY:HA2	1:D:28:ASP:HB2	1.59	0.85
1:D:169:ARG:HG3	1:D:169:ARG:HH11	1.52	0.73
1:D:465:ASP:OD1	1:D:468:ARG:NH2	2.22	0.71
1:D:322:ARG:NH2	5:D:2021:HOH:O	2.25	0.69
1:B:770:GLU:N	1:B:770:GLU:OE1	2.25	0.68
1:D:440:PHE:O	1:D:443:ASN:ND2	2.28	0.66
1:D:801:LEU:HG	1:D:837:LEU:HD11	1.78	0.65
1:B:322:ARG:NH2	5:B:2025:HOH:O	2.29	0.65
1:B:769:ILE:HG22	1:B:770:GLU:HA	1.79	0.65
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.81	0.63
1:D:440:PHE:N	1:D:443:ASN:OD1	2.29	0.62
1:D:54:VAL:HG11	1:D:60:MET:HG3	1.82	0.62
1:B:226:THR:O	1:B:471:LYS:NZ	2.30	0.62
1:D:684:GLN:O	1:D:688:ARG:NH1	2.32	0.62
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.82	0.62
1:D:688:ARG:NH2	2:D:1887:ATP:O1G	2.30	0.61
1:B:154:ILE:HB	1:B:162:VAL:HB	1.81	0.60
1:D:154:ILE:HB	1:D:162:VAL:HB	1.83	0.60
1:D:678:ARG:NH1	1:D:711:SER:OG	2.34	0.60
1:B:298:LYS:O	1:B:301:SER:OG	2.21	0.58
1:B:65:ARG:HG3	1:B:81:TRP:CD2	2.39	0.58
1:B:110:ASP:HB2	1:B:118:LEU:HD21	1.86	0.57
1:B:313:LYS:NZ	1:B:409:GLU:OE1	2.32	0.57
1:B:443:ASN:HB3	1:B:718:LEU:HD11	1.86	0.57
1:D:309:THR:HA	1:D:313:LYS:HE2	1.86	0.56
1:B:13:ASN:HD22	1:B:13:ASN:N	2.04	0.56
1:B:89:LEU:O	1:B:99:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:LYS:NZ	1:D:409:GLU:OE1	2.37	0.55
1:D:54:VAL:HG11	1:D:60:MET:CG	2.37	0.55
1:B:44:LEU:HD13	1:B:136:ILE:HG21	1.89	0.54
1:B:54:VAL:HG11	1:B:60:MET:HG3	1.90	0.53
1:B:688:ARG:NH2	2:B:1887:ATP:O1G	2.34	0.53
1:B:824:VAL:HG13	1:B:828:LYS:HB3	1.89	0.53
1:B:838:PRO:HG2	1:B:843:ILE:HD11	1.92	0.52
1:D:189:ASN:HA	1:D:192:ASN:OD1	2.10	0.51
1:B:801:LEU:HG	1:B:837:LEU:HD11	1.91	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.38	0.51
1:B:54:VAL:HG11	1:B:60:MET:CG	2.41	0.51
1:B:204:SER:HB2	1:B:209:THR:HG23	1.94	0.50
1:D:325:THR:HG21	1:D:378:ILE:HB	1.94	0.50
1:D:88:TYR:CE1	1:D:109:CYS:HB2	2.47	0.49
1:D:125:ASP:OD2	1:D:131:ARG:NH1	2.45	0.49
1:B:686:PHE:CZ	1:B:702:ILE:HG21	2.49	0.48
1:D:110:ASP:HB2	1:D:118:LEU:HD21	1.95	0.48
1:B:26:THR:OG1	1:B:27:GLY:HA2	2.13	0.48
1:D:679:TYR:CD1	1:D:718:LEU:HD12	2.49	0.48
1:B:256:VAL:HA	1:B:260:TYR:HB2	1.94	0.47
1:D:581:SER:O	1:D:597:GLU:HB3	2.15	0.47
1:D:528:THR:OG1	1:D:530:ARG:HD2	2.14	0.46
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.48	0.46
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.96	0.46
1:B:112:ILE:HD13	1:B:118:LEU:HD23	1.98	0.46
1:D:531:THR:HG23	1:D:532:PHE:H	1.80	0.46
1:D:441:PRO:HB2	1:D:442:GLU:HB2	1.98	0.46
1:D:825:ASP:O	1:D:828:LYS:HB2	2.15	0.46
1:D:224:ASP:N	1:D:224:ASP:OD1	2.48	0.46
1:D:838:PRO:HG2	1:D:843:ILE:HD11	1.98	0.46
1:D:686:PHE:CZ	1:D:702:ILE:HG21	2.52	0.45
1:D:328:ASP:OD1	1:D:329:PHE:N	2.49	0.45
1:B:684:GLN:O	1:B:688:ARG:NH1	2.47	0.45
1:D:89:LEU:HD21	1:D:159:LEU:HD21	1.98	0.44
1:D:354:SER:HB3	1:D:357:SER:OG	2.17	0.44
1:D:637:TYR:O	1:D:641:LEU:HB2	2.18	0.44
1:B:342:LEU:O	1:B:638:TYR:OH	2.32	0.44
1:B:57:GLN:OE1	1:B:192:ASN:HB3	2.17	0.44
1:B:637:TYR:O	1:B:641:LEU:HB2	2.18	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.52	0.44
1:B:440:PHE:N	1:B:443:ASN:OD1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ALA:HB1	1:D:203:ILE:HD11	1.99	0.43
1:B:704:THR:HG21	1:B:708:LEU:HD12	2.01	0.43
1:B:769:ILE:CG2	1:B:770:GLU:HA	2.46	0.43
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.52	0.43
1:D:204:SER:HB2	1:D:209:THR:HG23	1.99	0.43
1:D:57:GLN:HB2	1:D:191:GLU:O	2.19	0.43
1:B:60:MET:HE2	1:B:194:LEU:HD13	2.01	0.43
1:D:394:SER:HA	1:D:425:LYS:NZ	2.33	0.43
1:D:839:ALA:O	1:D:843:ILE:HG12	2.19	0.43
1:B:763:PHE:HA	1:B:768:SER:CB	2.49	0.43
1:B:544:VAL:HA	1:B:674:ASP:O	2.19	0.42
1:D:60:MET:HE1	1:D:160:PRO:HD3	2.02	0.42
1:D:490:GLU:HG2	1:D:512:ARG:HH21	1.83	0.42
1:B:763:PHE:HA	1:B:768:SER:HB3	2.01	0.42
1:D:44:LEU:HD13	1:D:136:ILE:HG21	2.02	0.42
1:B:640:ASP:OD2	1:B:644:ARG:NE	2.50	0.41
1:D:40:LEU:HD11	1:D:164:ILE:HG21	2.01	0.41
1:B:847:ARG:NH2	1:B:886:GLN:OE1	2.40	0.41
1:D:65:ARG:HG3	1:D:81:TRP:CD2	2.54	0.41
1:D:476:LYS:NZ	1:D:478:ASP:OD2	2.48	0.41
1:B:679:TYR:CD1	1:B:718:LEU:HD12	2.56	0.40
1:B:60:MET:HE1	1:B:160:PRO:HD3	2.03	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	B	827/1038 (80%)	798 (96%)	26 (3%)	3 (0%)	38	65
1	D	825/1038 (80%)	785 (95%)	37 (4%)	3 (0%)	38	65
All	All	1652/2076 (80%)	1583 (96%)	63 (4%)	6 (0%)	38	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	810	SER
1	B	807	ILE
1	B	810	SER
1	D	807	ILE
1	B	769	ILE
1	D	769	ILE

### 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	B	690/927 (74%)	656 (95%)	34 (5%)	29	56
1	D	684/927 (74%)	647 (95%)	37 (5%)	26	51
All	All	1374/1854 (74%)	1303 (95%)	71 (5%)	27	53

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	65	ARG
1	B	71	LEU
1	B	89	LEU
1	B	118	LEU
1	B	165	GLU
1	B	169	ARG
1	B	221	ASN
1	B	240	LEU
1	B	253	LEU
1	B	282	ARG
1	B	298	LYS
1	B	301	SER
1	B	307	HIS
1	B	332	LYS

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Mol	Chain	Res	Type
1	B	336	VAL
1	B	346	THR
1	B	356	ASP
1	B	393	GLU
1	B	402	GLN
1	B	422	LEU
1	B	464	THR
1	B	641	LEU
1	B	652	LEU
1	B	655	VAL
1	B	688	ARG
1	B	718	LEU
1	B	722	LYS
1	B	731	LYS
1	B	765	ASP
1	B	781	LEU
1	B	840	ASP
1	D	21	ILE
1	D	26	THR
1	D	40	LEU
1	D	89	LEU
1	D	118	LEU
1	D	134	VAL
1	D	163	GLN
1	D	192	ASN
1	D	217	LYS
1	D	224	ASP
1	D	240	LEU
1	D	253	LEU
1	D	307	HIS
1	D	309	THR
1	D	336	VAL
1	D	356	ASP
1	D	393	GLU
1	D	402	GLN
1	D	422	LEU
1	D	425	LYS
1	D	443	ASN
1	D	464	THR
1	D	532	PHE
1	D	581	SER
1	D	626	ASN

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Mol	Chain	Res	Type
1	D	641	LEU
1	D	647	ASN
1	D	652	LEU
1	D	655	VAL
1	D	688	ARG
1	D	710	ARG
1	D	718	LEU
1	D	731	LYS
1	D	765	ASP
1	D	781	LEU
1	D	805	GLN
1	D	854	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z  > 2$
2	ATP	B	1887	4	27,33,33	0.95	1 (3%)	25,52,52	1.59	2 (8%)
3	PO4	B	1888	-	4,4,4	0.74	0	6,6,6	0.38	0
3	PO4	B	1889	-	4,4,4	0.78	0	6,6,6	0.33	0
2	ATP	D	1887	4	27,33,33	0.94	1 (3%)	25,52,52	1.60	2 (8%)
3	PO4	D	1889	-	4,4,4	0.76	0	6,6,6	0.34	0
3	PO4	D	1890	-	4,4,4	0.81	0	6,6,6	0.40	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
2	ATP	B	1887	4	-	0/18/38/38	0/3/3/3
3	PO4	B	1888	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1889	-	-	0/0/0/0	0/0/0/0
2	ATP	D	1887	4	-	0/18/38/38	0/3/3/3
3	PO4	D	1889	-	-	0/0/0/0	0/0/0/0
3	PO4	D	1890	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1887	ATP	C5-C4	2.99	1.47	1.40
2	B	1887	ATP	C5-C4	2.99	1.47	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1887	ATP	N3-C2-N1	-5.97	123.66	128.86
2	B	1887	ATP	N3-C2-N1	-5.76	123.84	128.86
2	B	1887	ATP	C4-C5-N7	-2.78	106.73	109.41
2	D	1887	ATP	C4-C5-N7	-2.73	106.78	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1887	ATP	1	0
2	D	1887	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	B	837/1038 (80%)	0.79	97 (11%) 5 4	13, 33, 71, 121	0
1	D	835/1038 (80%)	0.93	133 (15%) 2 2	17, 40, 84, 114	0
All	All	1672/2076 (80%)	0.86	230 (13%) 3 3	13, 36, 78, 121	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	809	LEU	14.2
1	B	808	ASP	8.1
1	B	807	ILE	7.9
1	B	813	VAL	7.9
1	D	604	MET	7.6
1	D	534	GLY	7.4
1	D	566	ASN	7.3
1	D	809	LEU	7.3
1	D	768	SER	7.1
1	B	566	ASN	7.0
1	B	745	THR	6.8
1	B	814	ALA	6.8
1	B	812	PRO	6.7
1	D	533	PRO	6.5
1	D	818	PHE	6.5
1	D	816	GLU	6.4
1	D	808	ASP	6.1
1	D	565	ALA	6.0
1	B	564	ALA	6.0
1	B	568	SER	6.0
1	D	569	ALA	5.9
1	B	567	LYS	5.9
1	B	506	ALA	5.8
1	D	570	THR	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	820	ALA	5.5
1	D	603	ALA	5.5
1	D	819	LYS	5.3
1	D	769	ILE	5.1
1	D	563	GLU	5.0
1	D	807	ILE	5.0
1	D	813	VAL	5.0
1	B	498	LEU	5.0
1	D	767	THR	4.8
1	B	170	GLY	4.8
1	B	826	ASP	4.7
1	D	773	LYS	4.7
1	D	811	ASP	4.6
1	D	506	ALA	4.6
1	D	853	ILE	4.6
1	D	495	GLU	4.5
1	D	814	ALA	4.5
1	B	855	ASP	4.5
1	D	511	MET	4.4
1	D	623	PHE	4.4
1	D	441	PRO	4.4
1	B	604	MET	4.3
1	D	772	GLU	4.3
1	D	815	VAL	4.3
1	B	565	ALA	4.3
1	D	810	SER	4.2
1	D	562	GLU	4.2
1	B	722	LYS	4.2
1	D	855	ASP	4.1
1	B	723	ASN	4.1
1	B	511	MET	4.1
1	D	717	THR	4.1
1	B	744	ALA	4.1
1	D	723	ASN	4.0
1	B	818	PHE	4.0
1	D	567	LYS	4.0
1	D	535	SER	3.9
1	B	606	SER	3.9
1	B	718	LEU	3.8
1	D	502	GLU	3.8
1	D	421	ASN	3.8
1	B	621	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	714	ASP	3.8
1	D	774	GLU	3.8
1	D	743	ALA	3.8
1	D	499	SER	3.8
1	D	568	SER	3.7
1	D	582	PHE	3.7
1	B	494	ASP	3.7
1	D	571	TYR	3.7
1	B	356	ASP	3.7
1	B	571	TYR	3.6
1	D	564	ALA	3.6
1	D	355	PRO	3.6
1	D	602	SER	3.6
1	D	479	TYR	3.5
1	D	560	LEU	3.5
1	B	563	GLU	3.5
1	D	498	LEU	3.5
1	B	819	LYS	3.4
1	B	827	GLU	3.4
1	B	508	LEU	3.4
1	D	744	ALA	3.4
1	D	406	ILE	3.3
1	B	570	THR	3.3
1	B	502	GLU	3.3
1	D	820	ALA	3.3
1	B	824	VAL	3.3
1	B	825	ASP	3.3
1	B	496	LYS	3.3
1	D	764	PRO	3.3
1	D	765	ASP	3.3
1	D	817	LYS	3.2
1	D	365	ALA	3.2
1	B	509	HIS	3.2
1	D	745	THR	3.2
1	B	854	ARG	3.2
1	B	290	SER	3.1
1	D	374	ASP	3.1
1	B	618	GLU	3.1
1	D	601	THR	3.1
1	D	622	HIS	3.1
1	B	445	LEU	3.1
1	D	387	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	743	ALA	3.1
1	B	446	GLY	3.1
1	D	170	GLY	3.1
1	B	449	THR	3.1
1	D	572	LYS	3.1
1	D	806	GLN	3.0
1	D	679	TYR	3.0
1	D	505	GLN	3.0
1	D	500	ALA	3.0
1	D	812	PRO	3.0
1	B	806	GLN	3.0
1	B	742	ASP	3.0
1	B	444	ALA	3.0
1	B	770	GLU	3.0
1	D	822	HIS	3.0
1	D	605	ASP	3.0
1	B	357	SER	2.9
1	D	440	PHE	2.9
1	D	824	VAL	2.9
1	B	150	TYR	2.9
1	D	344	TYR	2.9
1	B	441	PRO	2.9
1	B	605	ASP	2.9
1	D	766	PRO	2.9
1	D	501	ALA	2.9
1	D	606	SER	2.9
1	D	850	TYR	2.9
1	D	295	ASN	2.9
1	B	623	PHE	2.8
1	B	829	PHE	2.8
1	D	32	SER	2.8
1	B	190	SER	2.7
1	D	508	LEU	2.7
1	D	763	PHE	2.7
1	D	721	ASP	2.7
1	D	852	ASP	2.7
1	B	355	PRO	2.7
1	B	535	SER	2.7
1	B	627	PHE	2.7
1	D	375	ASP	2.7
1	B	291	PHE	2.6
1	D	770	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	533	PRO	2.6
1	B	505	GLN	2.6
1	D	444	ALA	2.6
1	B	447	SER	2.5
1	B	817	LYS	2.5
1	B	534	GLY	2.5
1	D	493	THR	2.5
1	D	496	LYS	2.5
1	D	608	ALA	2.5
1	D	28	ASP	2.5
1	B	501	ALA	2.5
1	B	874	ASP	2.4
1	D	515	GLU	2.4
1	D	821	GLU	2.4
1	B	811	ASP	2.4
1	D	416	GLY	2.4
1	B	560	LEU	2.4
1	B	620	ASN	2.4
1	B	626	ASN	2.4
1	D	189	ASN	2.4
1	D	356	ASP	2.4
1	D	747	GLU	2.4
1	D	364	THR	2.4
1	D	447	SER	2.4
1	D	410	CYS	2.4
1	D	650	ILE	2.4
1	B	375	ASP	2.3
1	B	852	ASP	2.3
1	D	388	ASN	2.3
1	B	541	MET	2.3
1	D	618	GLU	2.3
1	D	110	ASP	2.3
1	B	189	ASN	2.3
1	D	531	THR	2.3
1	B	420	LYS	2.3
1	D	856	TRP	2.2
1	B	218	ARG	2.2
1	D	838	PRO	2.2
1	D	536	LYS	2.2
1	D	21	ILE	2.2
1	D	489	LEU	2.2
1	B	292	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	661	THR	2.2
1	D	760	GLU	2.2
1	D	851	ASN	2.2
1	B	721	ASP	2.2
1	D	293	ALA	2.2
1	D	598	THR	2.2
1	B	572	LYS	2.2
1	D	414	GLN	2.2
1	D	561	GLN	2.2
1	B	219	ASP	2.2
1	B	717	THR	2.2
1	B	856	TRP	2.2
1	D	321	ALA	2.2
1	D	832	LEU	2.1
1	B	581	SER	2.1
1	D	452	SER	2.1
1	D	614	ALA	2.1
1	D	449	THR	2.1
1	B	289	SER	2.1
1	B	769	ILE	2.1
1	D	494	ASP	2.1
1	D	825	ASP	2.1
1	B	495	GLU	2.1
1	B	816	GLU	2.1
1	D	285	TRP	2.1
1	D	445	LEU	2.1
1	B	751	GLY	2.1
1	B	660	LEU	2.1
1	D	559	ARG	2.1
1	D	581	SER	2.1
1	D	649	ASP	2.1
1	B	815	VAL	2.0
1	B	851	ASN	2.0
1	B	828	LYS	2.0
1	D	621	SER	2.0
1	D	859	ARG	2.0
1	B	830	ALA	2.0
1	D	422	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PO4	D	1889	5/5	0.86	0.17	-0.41	36,53,55,82	0
3	PO4	B	1889	5/5	0.90	0.16	-0.61	52,55,69,83	0
3	PO4	D	1890	5/5	0.98	0.14	-1.03	16,17,21,23	0
2	ATP	D	1887	31/31	0.97	0.17	-1.09	13,21,27,33	0
2	ATP	B	1887	31/31	0.97	0.16	-1.33	11,18,23,25	0
3	PO4	B	1888	5/5	0.98	0.13	-1.37	24,24,27,32	0
4	MG	B	1890	1/1	0.92	0.34	-	23,23,23,23	0
4	MG	D	1886	1/1	0.87	0.27	-	25,25,25,25	0

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

There are no such residues in this entry.