



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:35 PM BST

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

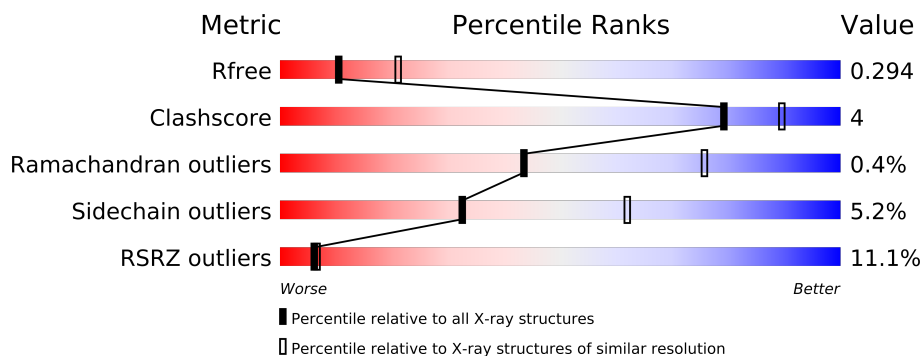
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

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}	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	B	1038	
1	D	1038	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	PO4	B	1889	-	X
4	MG	B	1890	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 13387 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

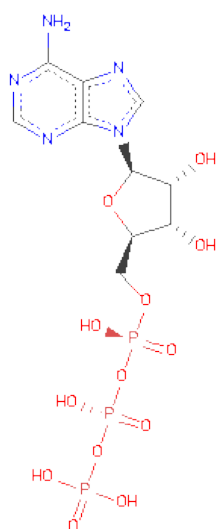
- Molecule 1 is a protein called TYPE I RESTRICTION ENZYME ECOR124II R PROTEIN.

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



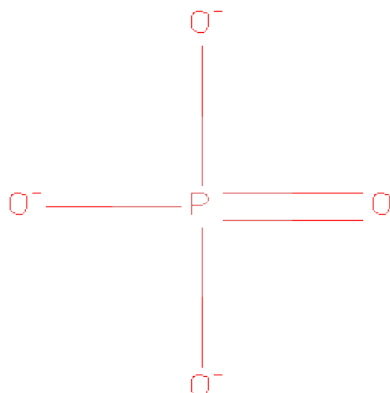
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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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: O₄P).



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.76Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.292 0.251 , 0.294	Depositor DCC
R_{free} test set	3192 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 33.6	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 63146 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13387	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6631	0	6305	44	0
1	D	6594	0	6268	47	0
2	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	12	1	0
3	B	10	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (91) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:89:LEU:O	1:B:99:LYS:NZ	2.38	0.56
1:B:13:ASN:HD22	1:B:13:ASN:N	2.04	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(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:54:VAL:HG11	1:B:60:MET:CG	2.41	0.51
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.38	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:825:ASP:O	1:D:828:LYS:HB2	2.15	0.46
1:D:441:PRO:HB2	1:D:442:GLU:HB2	1.98	0.46
1:D:838:PRO:HG2	1:D:843:ILE:HD11	1.98	0.46
1:D:224:ASP:N	1:D:224:ASP:OD1	2.48	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:637:TYR:O	1:D:641:LEU:HB2	2.18	0.44
1:D:354:SER:HB3	1:D:357:SER:OG	2.17	0.44
1:B:342:LEU:O	1:B:638:TYR:OH	2.32	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CZ	2.52	0.44
1:B:637:TYR:O	1:B:641:LEU:HB2	2.18	0.44
1:B:57:GLN:OE1	1:B:192:ASN:HB3	2.17	0.44
1:B:440:PHE:N	1:B:443:ASN:OD1	2.50	0.43
1:D:176:ALA:HB1	1:D:203:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:704:THR:HG21	1:B:708:LEU:HD12	2.01	0.43
1:D:57:GLN:HB2	1:D:191:GLU:O	2.19	0.43
1:D:204:SER:HB2	1:D:209:THR:HG23	1.99	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:D:40:LEU:HD11	1:D:164:ILE:HG21	2.01	0.41
1:B:640:ASP:OD2	1:B:644:ARG:NE	2.50	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%)	43	76
1	D	825/1038 (80%)	785 (95%)	37 (4%)	3 (0%)	43	76
All	All	1652/2076 (80%)	1583 (96%)	63 (4%)	6 (0%)	43	76

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%)	35	66
1	D	684/927 (74%)	647 (95%)	37 (5%)	31	60
All	All	1374/1854 (74%)	1303 (95%)	71 (5%)	32	62

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
1	B	336	VAL
1	B	346	THR
1	B	356	ASP

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Mol	Chain	Res	Type
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
1	D	641	LEU
1	D	647	ASN
1	D	652	LEU

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Mol	Chain	Res	Type
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 chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	33,33,33	1.02	2 (6%)	52,52,52	1.74	8 (15%)
3	PO4	B	1888	-	4,4,4	0.27	0	6,6,6	0.31	0
3	PO4	B	1889	-	4,4,4	0.29	0	6,6,6	0.31	0
2	ATP	D	1887	4	33,33,33	1.02	2 (6%)	52,52,52	1.77	10 (19%)
3	PO4	D	1889	-	4,4,4	0.26	0	6,6,6	0.31	0
3	PO4	D	1890	-	4,4,4	0.30	0	6,6,6	0.31	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	-	0/22/38/38	0/1/3/3
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	-	0/22/38/38	0/1/3/3
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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1887	ATP	C5-C4	2.99	1.47	1.40
2	D	1887	ATP	C5-C4	2.99	1.47	1.40
2	D	1887	ATP	C4-N9	-2.74	1.33	1.37
2	B	1887	ATP	C4-N9	-2.72	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1887	ATP	N3-C2-N1	-6.04	123.66	128.71
2	B	1887	ATP	N3-C2-N1	-5.82	123.84	128.71
2	B	1887	ATP	N3-C4-N9	5.42	135.22	125.43
2	D	1887	ATP	N3-C4-N9	5.37	135.12	125.43
2	B	1887	ATP	PA-O3A-PB	-3.89	120.28	131.68
2	D	1887	ATP	PA-O3A-PB	-3.67	120.91	131.68
2	B	1887	ATP	C4-C5-N7	-3.26	106.73	109.52
2	D	1887	ATP	C4-C5-N7	-3.20	106.78	109.52
2	B	1887	ATP	C5-C4-N3	-3.17	118.80	125.70
2	D	1887	ATP	C5-C4-N3	-3.15	118.83	125.70
2	D	1887	ATP	O4'-C1'-N9	3.02	111.25	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1887	ATP	PB-O3B-PG	-2.79	123.49	131.68
2	B	1887	ATP	PB-O3B-PG	-2.74	123.66	131.68
2	B	1887	ATP	C8-N9-C4	2.57	108.86	106.90
2	D	1887	ATP	C8-N9-C4	2.46	108.78	106.90
2	D	1887	ATP	C2-N3-C4	2.37	120.75	114.01
2	B	1887	ATP	C2-N3-C4	2.35	120.70	114.01
2	D	1887	ATP	C3'-C2'-C1'	2.07	104.14	100.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	837/1038 (80%)	0.57	77 (9%) 9 10	13, 33, 71, 121	0
1	D	835/1038 (80%)	0.77	110 (13%) 4 5	17, 40, 84, 114	0
All	All	1672/2076 (80%)	0.67	187 (11%) 6 6	13, 36, 78, 121	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	809	LEU	14.8
1	D	809	LEU	8.6
1	B	808	ASP	8.5
1	D	604	MET	8.2
1	D	534	GLY	8.2
1	D	566	ASN	7.8
1	B	566	ASN	7.3
1	B	807	ILE	7.2
1	B	745	THR	7.0
1	D	768	SER	7.0
1	B	813	VAL	6.9
1	D	808	ASP	6.8
1	D	533	PRO	6.6
1	D	563	GLU	6.5
1	D	565	ALA	6.4
1	B	812	PRO	6.3
1	D	603	ALA	6.3
1	D	818	PHE	6.2
1	B	564	ALA	6.1
1	B	567	LYS	6.0
1	D	811	ASP	5.9
1	D	807	ILE	5.9
1	B	814	ALA	5.6
1	D	816	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	769	ILE	5.4
1	D	819	LYS	5.3
1	D	562	GLU	5.2
1	D	810	SER	5.1
1	B	498	LEU	5.1
1	D	570	THR	5.1
1	B	565	ALA	5.0
1	D	714	ASP	5.0
1	D	560	LEU	4.9
1	B	170	GLY	4.9
1	D	535	SER	4.8
1	D	569	ALA	4.8
1	D	814	ALA	4.7
1	D	813	VAL	4.6
1	D	767	THR	4.5
1	D	623	PHE	4.5
1	B	568	SER	4.4
1	D	815	VAL	4.4
1	D	773	LYS	4.3
1	B	744	ALA	4.3
1	D	502	GLU	4.3
1	B	820	ALA	4.2
1	D	511	MET	4.2
1	B	855	ASP	4.1
1	D	421	ASN	4.0
1	B	534	GLY	4.0
1	B	722	LYS	4.0
1	D	743	ALA	4.0
1	B	818	PHE	3.9
1	B	604	MET	3.9
1	D	441	PRO	3.9
1	B	506	ALA	3.9
1	B	621	SER	3.8
1	B	827	GLU	3.8
1	D	498	LEU	3.8
1	D	770	GLU	3.7
1	D	479	TYR	3.7
1	D	679	TYR	3.7
1	B	718	LEU	3.7
1	D	774	GLU	3.7
1	D	564	ALA	3.7
1	D	772	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	494	ASP	3.6
1	B	826	ASP	3.6
1	B	535	SER	3.6
1	B	563	GLU	3.6
1	D	602	SER	3.5
1	D	812	PRO	3.5
1	D	650	ILE	3.5
1	D	571	TYR	3.4
1	B	770	GLU	3.4
1	B	618	GLU	3.4
1	D	606	SER	3.4
1	D	582	PHE	3.4
1	B	819	LYS	3.4
1	B	447	SER	3.4
1	B	571	TYR	3.3
1	D	744	ALA	3.3
1	B	502	GLU	3.3
1	B	606	SER	3.3
1	B	811	ASP	3.3
1	D	601	THR	3.3
1	B	743	ALA	3.3
1	D	365	ALA	3.2
1	D	506	ALA	3.2
1	B	189	ASN	3.2
1	B	508	LEU	3.2
1	D	765	ASP	3.2
1	D	495	GLU	3.2
1	B	627	PHE	3.1
1	D	605	ASP	3.1
1	B	511	MET	3.1
1	B	290	SER	3.1
1	D	806	GLN	3.1
1	D	622	HIS	3.0
1	B	623	PHE	3.0
1	B	449	THR	3.0
1	D	717	THR	2.9
1	D	559	ARG	2.9
1	B	375	ASP	2.9
1	B	533	PRO	2.9
1	B	806	GLN	2.9
1	D	536	LYS	2.9
1	D	387	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	376	ASN	2.9
1	D	745	THR	2.9
1	D	723	ASN	2.8
1	B	496	LYS	2.8
1	B	854	ARG	2.8
1	D	763	PHE	2.8
1	B	446	GLY	2.8
1	B	625	THR	2.8
1	B	723	ASN	2.8
1	D	766	PRO	2.8
1	D	32	SER	2.8
1	D	567	LYS	2.7
1	D	561	GLN	2.7
1	B	742	ASP	2.7
1	D	295	ASN	2.7
1	D	853	ILE	2.7
1	B	190	SER	2.6
1	D	388	ASN	2.6
1	D	489	LEU	2.6
1	B	445	LEU	2.6
1	D	374	ASP	2.6
1	D	410	CYS	2.5
1	D	820	ALA	2.5
1	B	560	LEU	2.5
1	D	805	GLN	2.5
1	B	810	SER	2.5
1	B	605	ASP	2.5
1	B	620	ASN	2.5
1	D	499	SER	2.5
1	D	447	SER	2.5
1	B	626	ASN	2.5
1	D	344	TYR	2.5
1	D	627	PHE	2.4
1	D	508	LEU	2.4
1	D	804	LEU	2.4
1	B	444	ALA	2.4
1	D	649	ASP	2.4
1	D	764	PRO	2.4
1	D	822	HIS	2.4
1	B	441	PRO	2.3
1	B	291	PHE	2.3
1	D	635	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	817	LYS	2.3
1	D	568	SER	2.3
1	D	621	SER	2.3
1	B	356	ASP	2.3
1	D	855	ASP	2.3
1	B	541	MET	2.3
1	B	825	ASP	2.3
1	D	721	ASP	2.3
1	D	618	GLU	2.3
1	B	292	THR	2.2
1	B	721	ASP	2.2
1	D	850	TYR	2.2
1	B	821	GLU	2.2
1	B	874	ASP	2.2
1	D	21	ILE	2.2
1	B	611	PHE	2.2
1	D	493	THR	2.2
1	D	97	LEU	2.2
1	B	357	SER	2.1
1	D	747	GLU	2.1
1	D	445	LEU	2.1
1	D	355	PRO	2.1
1	D	760	GLU	2.1
1	B	829	PHE	2.1
1	D	655	VAL	2.1
1	D	375	ASP	2.1
1	D	608	ALA	2.1
1	D	440	PHE	2.1
1	D	505	GLN	2.1
1	D	190	SER	2.1
1	D	406	ILE	2.1
1	B	509	HIS	2.0
1	D	821	GLU	2.0
1	D	95	GLY	2.0
1	D	191	GLU	2.0
1	B	769	ILE	2.0
1	D	31	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	B	1890	1/1	0.22	3.75	23,23,23,23	0
3	PO4	B	1889	5/5	0.18	2.29	52,55,69,83	0
4	MG	D	1886	1/1	0.19	0.49	25,25,25,25	0
3	PO4	D	1889	5/5	0.16	0.12	36,53,55,82	0
3	PO4	D	1890	5/5	0.12	-0.95	16,17,21,23	0
2	ATP	D	1887	31/31	0.14	-1.01	13,21,27,33	0
2	ATP	B	1887	31/31	0.13	-1.57	11,18,23,25	0
3	PO4	B	1888	5/5	0.10	-1.66	24,24,27,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.