



Full wwPDB X-ray Structure Validation 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
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Deposited on : 2013-03-07
Resolution : 2.99 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 ⓘ 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

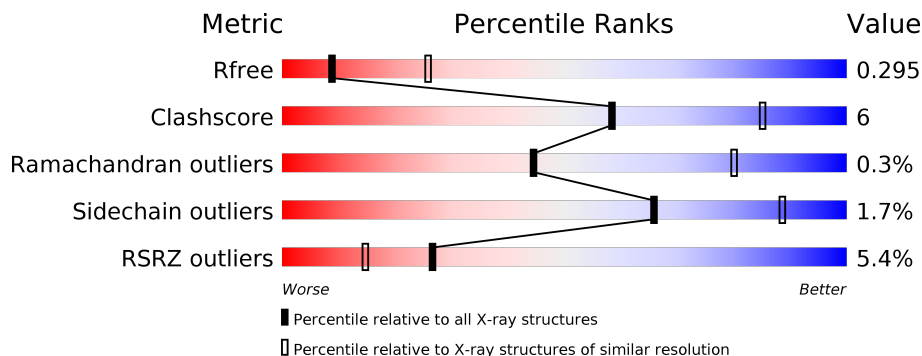
1 Overall quality at a glance

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			

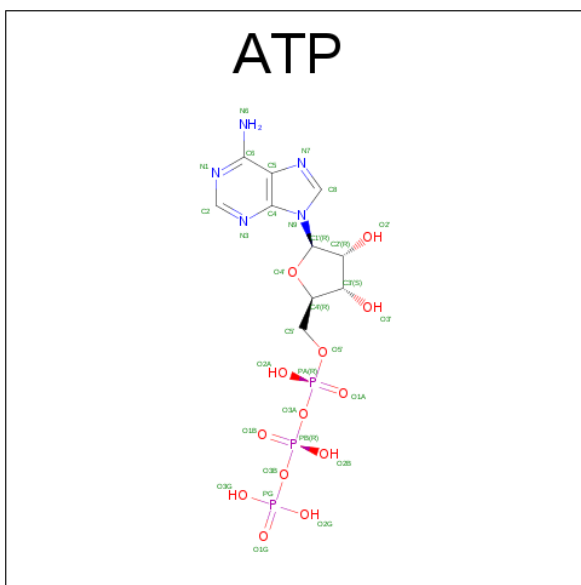
There are 4 discrepancies between the modelled and reference sequences:

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

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
LYS
ILE

● Molecule 1: TYPE I RESTRICTION ENZYME HSDR



VAL	PHE	GLN	PHE	GLN	GLN	HIS	D808	GLY	K427	D264	R149	MET	THR	THR	HIS	GLN	THR	HIS	THR	ILE	ALA	GLU	SER	ASN	N13	F14	I15	D18	I21	T26	G27	D28	S29	L36	L40	Q57	N63	Q67	Y88	L89	K99	K102	D106	F113	E116	R117	L118	E119	F140	GLU	GLN	ALA	GLY	SER	HIS	ALA	ASN																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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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.*

¹ Intensities estimated from amplitudes.

² 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

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	0.27	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.

All (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
1	B	769	ILE	Peptide
1	B	806	GLN	Peptide
1	B	812	PRO	Peptide
1	C	769	ILE	Peptide
1	C	806	GLN	Peptide
1	D	769	ILE	Peptide
1	D	811	ASP	Peptide
1	D	812	PRO	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.

All (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
1:A:365:ALA:HB3	1:C:116:GLU:HB3	1.65	0.79
1:D:819:LYS:NZ	1:D:826:ASP:OD1	2.17	0.78
1:A:810:SER:HB3	1:A:812:PRO:HD3	1.67	0.76
1:B:810:SER:HB3	1:B:812:PRO:HD3	1.65	0.76
1:D:807:ILE:H	1:D:808:ASP:HB2	1.50	0.75
1:A:213:ALA:HB2	1:A:271:VAL:HG23	1.69	0.74
1:B:116:GLU:HB3	1:D:365:ALA:HB3	1.68	0.74
1:C:851:ASN:OD1	1:C:854:ARG:NH1	2.22	0.72
1:D:769:ILE:HG22	1:D:770:GLU:HA	1.70	0.72
1:A:807:ILE:N	1:A:808:ASP:HB2	2.05	0.71
1:C:810:SER:HB3	1:C:812:PRO:HD3	1.74	0.70
1:C:881:ASP:N	1:C:881:ASP:OD1	2.23	0.69
1:A:583:ALA:HB2	1:A:597:GLU:HG2	1.73	0.69
1:A:116:GLU:HB3	1:C:365:ALA:HB3	1.75	0.68
1:C:57:GLN:HE22	1:C:194:LEU:H	1.42	0.68
1:B:541:MET:HG3	1:B:668:LEU:HD11	1.76	0.67
1:B:807:ILE:N	1:B:808:ASP:HB2	2.09	0.67
1:A:94:ASP:OD2	1:A:102:LYS:NZ	2.27	0.66
1:B:125:ASP:OD2	1:B:131:ARG:NH1	2.27	0.66
1:D:154:ILE:HB	1:D:162:VAL:HB	1.75	0.66
1:A:811:ASP:H	1:A:814:ALA:HB3	1.60	0.66
1:B:855:ASP:OD1	1:B:858:ARG:NH1	2.28	0.66
1:D:57:GLN:HE22	1:D:194:LEU:H	1.44	0.66
1:B:97:LEU:HD21	1:B:267:GLN:HB3	1.78	0.66
1:C:632:ASN:O	1:C:636:ASN:ND2	2.28	0.66
1:C:812:PRO:HB3	1:C:815:VAL:HB	1.78	0.66
1:A:313:LYS:NZ	1:A:409:GLU:OE2	2.30	0.65
1:B:811:ASP:H	1:B:814:ALA:HB3	1.61	0.65
1:D:532:PHE:O	1:D:534:GLY:HA3	1.97	0.65
1:B:365:ALA:HB3	1:D:116:GLU:HB3	1.78	0.65
1:C:807:ILE:N	1:C:808:ASP:HB2	2.11	0.65
1:B:265:SER:HB3	1:B:352:ARG:HE	1.61	0.64
1:A:632:ASN:O	1:A:636:ASN:ND2	2.30	0.64
1:C:213:ALA:HB2	1:C:271:VAL:HG23	1.79	0.64
1:B:313:LYS:NZ	1:B:409:GLU:OE2	2.30	0.64
1:B:89:LEU:HD11	1:B:159:LEU:HD21	1.79	0.63
1:C:395:ASP:HB3	1:D:836:ARG:HE	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASP:OD2	1:C:131:ARG:NH1	2.32	0.62
1:A:110:ASP:OD1	1:A:120:ASN:ND2	2.33	0.62
1:A:154:ILE:HB	1:A:162:VAL:HB	1.82	0.62
1:C:313:LYS:NZ	1:C:409:GLU:OE2	2.26	0.62
1:C:87:GLN:O	1:C:91:ASN:ND2	2.32	0.62
1:B:819:LYS:NZ	1:B:826:ASP:OD1	2.23	0.61
1:D:807:ILE:N	1:D:808:ASP:HB2	2.14	0.61
1:D:40:LEU:HD12	1:D:240:LEU:HD21	1.82	0.61
1:C:613:ASP:OD1	1:C:629:THR:OG1	2.13	0.61
1:B:554:TYR:HB3	1:B:611:PHE:HZ	1.66	0.60
1:A:755:VAL:HG13	1:A:781:LEU:HD22	1.83	0.60
1:B:297:SER:OG	1:B:427:LYS:O	2.14	0.60
1:B:854:ARG:NH2	1:B:858:ARG:HH22	2.00	0.60
1:A:554:TYR:HB3	1:A:611:PHE:HZ	1.67	0.60
1:B:204:SER:HB2	1:B:209:THR:HG23	1.84	0.60
1:D:213:ALA:HB2	1:D:271:VAL:HG23	1.83	0.59
1:D:755:VAL:HG13	1:D:781:LEU:HD22	1.84	0.59
1:D:741:THR:HA	1:D:748:ALA:HA	1.82	0.59
1:C:645:VAL:HG21	1:C:653:LEU:HD22	1.83	0.59
1:D:344:TYR:HA	1:D:639:ARG:CZ	2.33	0.59
1:D:541:MET:HG3	1:D:668:LEU:HD11	1.85	0.59
1:D:347:MET:HB2	1:D:639:ARG:NH2	2.17	0.59
1:A:851:ASN:OD1	1:A:854:ARG:NH1	2.35	0.58
1:A:91:ASN:OD1	1:A:91:ASN:N	2.34	0.58
1:C:244:THR:HA	1:C:248:PHE:HB2	1.86	0.57
1:A:763:PHE:HD1	1:A:768:SER:HB3	1.70	0.57
1:D:297:SER:OG	1:D:427:LYS:O	2.16	0.57
1:A:811:ASP:O	1:A:814:ALA:N	2.37	0.57
1:A:581:SER:HB3	1:A:597:GLU:HB3	1.87	0.56
1:D:117:ARG:NH1	1:D:119:GLU:OE2	2.38	0.56
1:B:854:ARG:HH21	1:B:858:ARG:HH22	1.52	0.56
1:B:812:PRO:HA	1:B:814:ALA:H	1.70	0.56
1:C:811:ASP:O	1:C:814:ALA:N	2.34	0.55
1:A:349:GLU:OE2	1:A:352:ARG:NH2	2.30	0.55
1:B:22:LYS:HG3	1:B:242:ASP:OD2	2.06	0.55
1:B:344:TYR:HD1	1:B:639:ARG:HG2	1.70	0.55
1:B:101:ARG:NH1	1:B:106:ASP:OD2	2.36	0.55
1:C:776:LYS:HG2	1:C:876:VAL:HG11	1.89	0.55
1:C:154:ILE:HB	1:C:162:VAL:HB	1.89	0.54
1:B:645:VAL:HG21	1:B:653:LEU:HD22	1.89	0.54
1:B:811:ASP:O	1:B:814:ALA:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:THR:HA	1:B:248:PHE:HB2	1.89	0.54
1:A:873:TRP:HE3	1:A:876:VAL:HG21	1.73	0.53
1:C:54:VAL:HG13	1:C:59:ALA:HB3	1.90	0.53
1:C:554:TYR:HB3	1:C:611:PHE:HZ	1.72	0.53
1:B:745:THR:O	1:B:747:GLU:HB2	2.09	0.53
1:D:769:ILE:CG2	1:D:770:GLU:HA	2.38	0.53
1:B:54:VAL:HG13	1:B:59:ALA:HB3	1.91	0.53
1:B:213:ALA:HB2	1:B:271:VAL:HG23	1.91	0.53
1:C:227:MET:HG2	1:C:273:ARG:HG2	1.89	0.53
1:B:162:VAL:HG22	1:B:200:LEU:HB3	1.92	0.52
1:B:462:VAL:HG23	1:B:465:ASP:H	1.73	0.52
1:C:812:PRO:HA	1:C:815:VAL:H	1.75	0.52
1:C:218:ARG:HA	1:C:219:ASP:C	2.30	0.51
1:D:462:VAL:HG23	1:D:465:ASP:H	1.75	0.51
1:D:482:VAL:HG23	1:D:483:ARG:HG3	1.93	0.51
1:C:806:GLN:CB	1:C:807:ILE:HA	2.41	0.51
1:A:490:GLU:HB3	1:A:706:ARG:HA	1.93	0.51
1:D:859:ARG:H	1:D:859:ARG:NH1	2.04	0.50
1:C:91:ASN:N	1:C:91:ASN:OD1	2.36	0.50
1:C:391:LYS:HD3	1:C:417:GLU:OE2	2.11	0.49
1:C:824:VAL:HG13	1:C:828:LYS:HB3	1.94	0.49
1:A:462:VAL:HG23	1:A:465:ASP:H	1.76	0.49
1:A:645:VAL:HG21	1:A:653:LEU:HD22	1.94	0.49
1:A:96:ILE:H	1:A:96:ILE:HD12	1.77	0.49
1:A:695:ALA:HB3	1:A:881:ASP:HB2	1.94	0.49
1:A:812:PRO:HA	1:A:814:ALA:H	1.78	0.49
1:D:804:LEU:HD23	1:D:818:PHE:CE2	2.47	0.49
1:B:154:ILE:HB	1:B:162:VAL:HB	1.94	0.49
1:A:147:ALA:HB1	1:A:148:ASN:CA	2.33	0.49
1:D:204:SER:HB2	1:D:209:THR:HG23	1.95	0.49
1:D:465:ASP:OD1	1:D:468:ARG:NH1	2.44	0.48
1:D:765:ASP:HB2	1:D:766:PRO:HA	1.94	0.48
1:A:303:GLY:O	1:A:432:PHE:HA	2.13	0.48
1:B:772:GLU:HG2	1:B:873:TRP:HE1	1.79	0.48
1:B:695:ALA:HB3	1:B:881:ASP:HB2	1.95	0.48
1:B:355:PRO:HD2	1:B:370:ASN:HD21	1.79	0.48
1:C:384:GLN:HG3	1:C:414:GLN:HG3	1.96	0.48
1:B:71:LEU:O	1:B:131:ARG:NH2	2.41	0.48
1:B:873:TRP:HE3	1:B:876:VAL:HG21	1.78	0.48
1:D:36:LEU:HB3	1:D:166:LEU:HD22	1.95	0.48
1:D:554:TYR:HB3	1:D:611:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:O	1:A:91:ASN:HB3	2.14	0.47
1:A:244:THR:HA	1:A:248:PHE:HB2	1.96	0.47
1:D:814:ALA:HA	1:D:817:LYS:HB3	1.94	0.47
1:A:125:ASP:OD2	1:A:131:ARG:NH1	2.47	0.47
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.70	0.47
1:C:162:VAL:HG22	1:C:200:LEU:HB3	1.96	0.47
1:D:384:GLN:HG3	1:D:414:GLN:HG3	1.96	0.47
1:B:772:GLU:HG3	1:B:856:TRP:HH2	1.78	0.47
1:D:770:GLU:O	1:D:775:LYS:NZ	2.48	0.47
1:B:833:GLN:O	1:B:836:ARG:NH2	2.48	0.47
1:B:36:LEU:HB3	1:B:166:LEU:HD22	1.96	0.47
1:C:13:ASN:N	1:C:13:ASN:HD22	2.11	0.47
1:D:313:LYS:NZ	1:D:409:GLU:OE2	2.48	0.47
1:D:806:GLN:CB	1:D:807:ILE:HA	2.45	0.46
1:A:36:LEU:HB3	1:A:166:LEU:HD22	1.97	0.46
1:D:264:ASP:HB2	1:D:349:GLU:OE1	2.15	0.46
1:D:15:ILE:HD11	1:D:277:ILE:HG21	1.96	0.46
1:D:89:LEU:HD11	1:D:159:LEU:HD21	1.97	0.46
1:A:63:ASN:O	1:A:67:GLN:HG2	2.15	0.46
1:C:297:SER:OG	1:C:427:LYS:O	2.21	0.46
1:D:303:GLY:O	1:D:432:PHE:HA	2.15	0.46
1:A:175:GLU:O	1:A:179:GLN:HG3	2.15	0.46
1:A:91:ASN:O	1:A:94:ASP:HB2	2.15	0.46
1:C:264:ASP:OD1	1:C:266:SER:OG	2.24	0.46
1:D:509:HIS:CE1	1:D:511:MET:HB2	2.51	0.46
1:A:807:ILE:HD13	1:A:807:ILE:HA	1.88	0.46
1:B:750:ARG:HH21	1:B:784:GLU:CD	2.19	0.46
1:D:582:PHE:H	1:D:604:MET:HG2	1.80	0.46
1:B:807:ILE:HA	1:B:807:ILE:HD13	1.90	0.46
1:D:298:LYS:HB2	1:D:300:GLU:HG2	1.97	0.46
1:A:57:GLN:HE21	1:A:57:GLN:HA	1.81	0.46
1:B:384:GLN:HG3	1:B:414:GLN:HG3	1.98	0.46
1:C:575:ARG:HD2	1:C:575:ARG:HA	1.71	0.46
1:C:792:LEU:HB3	1:C:798:PHE:CG	2.51	0.46
1:A:824:VAL:HG13	1:A:828:LYS:HB3	1.97	0.46
1:D:402:GLN:NE2	1:D:430:TYR:OH	2.47	0.46
1:B:393:GLU:HB3	1:B:396:LEU:HG	1.98	0.45
1:D:40:LEU:HD12	1:D:166:LEU:HD21	1.96	0.45
1:D:265:SER:HB3	1:D:352:ARG:HE	1.81	0.45
1:A:427:LYS:HA	1:A:427:LYS:HD3	1.75	0.45
1:A:71:LEU:O	1:A:131:ARG:NH2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:ILE:HG22	1:A:770:GLU:HA	1.98	0.45
1:C:691:ARG:HH22	3:C:1886:ATP:PG	2.40	0.45
1:D:256:VAL:HA	1:D:260:TYR:HB2	1.97	0.45
1:A:344:TYR:HD2	1:A:639:ARG:HG2	1.82	0.45
1:C:128:ASN:ND2	1:C:131:ARG:HG3	2.32	0.45
1:D:36:LEU:HD11	1:D:206:GLY:HA3	1.98	0.45
1:D:63:ASN:O	1:D:67:GLN:HG2	2.17	0.45
1:D:88:TYR:O	1:D:102:LYS:HE2	2.16	0.45
1:B:325:THR:HG21	1:B:378:ILE:HB	1.98	0.45
1:C:319:LYS:HD2	1:C:319:LYS:HA	1.76	0.45
1:A:750:ARG:NH1	1:A:758:GLU:OE1	2.50	0.45
1:B:851:ASN:HA	1:B:854:ARG:NH1	2.32	0.45
1:C:22:LYS:HG3	1:C:242:ASP:OD2	2.16	0.45
1:D:304:TYR:CZ	1:D:457:GLU:HB2	2.52	0.45
1:A:468:ARG:HD2	1:A:469:ASP:OD1	2.17	0.44
1:D:113:PHE:HE1	1:D:119:GLU:HB2	1.83	0.44
1:A:36:LEU:O	1:A:40:LEU:HB2	2.17	0.44
1:B:575:ARG:HD2	1:B:575:ARG:HA	1.71	0.44
1:C:162:VAL:HG21	1:C:253:LEU:HD11	2.00	0.44
1:D:873:TRP:HE3	1:D:876:VAL:HG21	1.82	0.44
1:A:296:TRP:NE1	1:A:428:ARG:HG2	2.32	0.44
1:A:471:LYS:HA	1:A:471:LYS:HD3	1.81	0.44
1:C:509:HIS:CE1	1:C:511:MET:HB2	2.52	0.44
1:D:102:LYS:HA	1:D:106:ASP:HB2	2.00	0.44
1:A:575:ARG:HA	1:A:575:ARG:HD2	1.74	0.44
1:D:40:LEU:HD11	1:D:164:ILE:HG21	1.99	0.44
1:B:99:LYS:HD2	1:B:197:TYR:CE2	2.53	0.43
1:B:683:MET:HG3	1:B:719:PHE:CD2	2.52	0.43
1:D:194:LEU:HA	1:D:194:LEU:HD23	1.91	0.43
1:D:683:MET:HG3	1:D:719:PHE:CD2	2.53	0.43
1:B:811:ASP:HA	1:B:812:PRO:HD3	1.76	0.43
1:B:13:ASN:N	1:B:13:ASN:OD1	2.49	0.43
1:B:229:TRP:CD1	1:B:247:CYS:HB2	2.54	0.43
1:B:304:TYR:CZ	1:B:457:GLU:HB2	2.53	0.43
1:B:88:TYR:CZ	1:B:109:CYS:HB2	2.53	0.43
1:C:40:LEU:HG	1:C:240:LEU:HD21	2.01	0.43
1:C:471:LYS:HA	1:C:471:LYS:HD3	1.88	0.43
1:B:427:LYS:HD3	1:B:427:LYS:HA	1.74	0.43
1:C:325:THR:HG21	1:C:378:ILE:HB	1.99	0.43
1:A:833:GLN:O	1:A:836:ARG:NH2	2.52	0.43
1:B:509:HIS:HA	1:B:510:PRO:HD3	1.94	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:ARG:NH2	1:B:777:ASP:HB3	2.34	0.43
1:D:18:ASP:HA	1:D:232:SER:OG	2.19	0.43
1:B:264:ASP:HB2	1:B:349:GLU:OE1	2.19	0.43
1:B:91:ASN:HB2	1:B:94:ASP:CG	2.39	0.43
1:C:303:GLY:O	1:C:432:PHE:HA	2.18	0.43
1:D:391:LYS:HD3	1:D:417:GLU:OE2	2.19	0.43
1:B:873:TRP:O	1:B:876:VAL:HG22	2.19	0.43
1:C:395:ASP:HB3	1:D:836:ARG:HB2	2.01	0.43
1:C:247:CYS:HA	1:C:252:THR:HG21	2.01	0.43
1:D:368:LYS:HB3	1:D:368:LYS:HE2	1.92	0.43
1:B:256:VAL:HA	1:B:260:TYR:HB2	2.00	0.42
1:D:855:ASP:O	1:D:858:ARG:NH1	2.52	0.42
1:A:227:MET:HG2	1:A:273:ARG:HG2	2.01	0.42
1:B:100:THR:HG23	1:B:199:GLN:OE1	2.19	0.42
1:B:368:LYS:HE2	1:B:368:LYS:HB3	1.77	0.42
1:D:873:TRP:O	1:D:876:VAL:HG22	2.20	0.42
1:A:15:ILE:HD11	1:A:277:ILE:HG21	2.01	0.42
1:A:167:LYS:HE3	1:A:176:ALA:HB1	2.01	0.42
1:A:40:LEU:HD12	1:A:166:LEU:HD21	2.01	0.42
1:D:280:THR:HG21	1:D:323:LEU:HD12	2.01	0.42
1:D:745:THR:O	1:D:747:GLU:N	2.52	0.42
1:A:575:ARG:HE	1:A:622:HIS:CG	2.38	0.42
1:A:684:GLN:O	1:A:688:ARG:NE	2.50	0.42
1:D:859:ARG:HD3	1:D:859:ARG:H	1.84	0.42
1:A:687:SER:HB2	1:A:688:ARG:HH21	1.84	0.42
1:A:704:THR:HG21	1:A:708:LEU:HD12	2.01	0.42
1:C:279:ALA:O	1:C:283:ILE:HG13	2.20	0.42
1:D:262:VAL:HG21	1:D:315:LEU:HD11	2.01	0.42
1:A:99:LYS:HD2	1:A:197:TYR:CE2	2.55	0.42
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.84	0.42
1:A:551:LYS:HA	1:A:611:PHE:CZ	2.55	0.42
1:A:850:TYR:CD2	1:A:883:LEU:HD11	2.54	0.42
1:B:337:VAL:O	1:B:382:THR:HA	2.20	0.42
1:B:303:GLY:O	1:B:432:PHE:HA	2.20	0.42
1:B:88:TYR:O	1:B:102:LYS:NZ	2.46	0.42
1:C:36:LEU:HB3	1:C:166:LEU:HD22	2.02	0.42
1:C:765:ASP:HB2	1:C:766:PRO:HA	2.01	0.42
1:C:36:LEU:O	1:C:40:LEU:HB2	2.20	0.41
1:C:755:VAL:HG13	1:C:781:LEU:HD22	2.01	0.41
1:A:467:ILE:HD13	1:A:474:LYS:HG2	2.02	0.41
1:B:490:GLU:HB3	1:B:706:ARG:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:LYS:HD3	1:C:427:LYS:HA	1.76	0.41
1:C:551:LYS:HG2	1:C:611:PHE:CG	2.55	0.41
1:A:509:HIS:CE1	1:A:511:MET:HB2	2.55	0.41
1:D:792:LEU:HB3	1:D:798:PHE:CG	2.55	0.41
1:A:507:PHE:O	1:A:512:ARG:NH1	2.49	0.41
1:D:772:GLU:OE2	1:D:873:TRP:NE1	2.42	0.41
1:A:89:LEU:HD11	1:A:159:LEU:HD21	2.01	0.41
1:A:30:TYR:HD2	1:A:169:ARG:HD3	1.85	0.41
1:A:54:VAL:HG13	1:A:59:ALA:HB3	2.01	0.41
1:B:102:LYS:HA	1:B:106:ASP:HB2	2.03	0.41
1:C:468:ARG:HD2	1:C:469:ASP:OD1	2.20	0.41
1:C:482:VAL:O	1:C:484:PRO:HD3	2.20	0.41
1:A:264:ASP:HB2	1:A:349:GLU:OE1	2.20	0.41
1:B:200:LEU:HD13	1:B:271:VAL:HG21	2.03	0.41
1:B:482:VAL:HG23	1:B:483:ARG:HG3	2.01	0.41
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.86	0.41
1:A:333:VAL:HG22	1:A:404:VAL:HB	2.02	0.41
1:B:516:ILE:HG23	1:B:705:PHE:CE1	2.56	0.41
1:D:171:VAL:O	1:D:205:ASN:ND2	2.40	0.41
1:D:21:ILE:H	1:D:21:ILE:HG12	1.64	0.41
1:A:273:ARG:N	1:A:276:GLN:OE1	2.49	0.41
1:A:283:ILE:O	1:A:287:ILE:HG13	2.20	0.41
1:A:412:ARG:HG2	1:A:439:ILE:HD11	2.03	0.41
1:A:391:LYS:HD3	1:A:417:GLU:OE2	2.21	0.41
1:A:482:VAL:O	1:A:484:PRO:HD3	2.21	0.41
1:C:482:VAL:HG23	1:C:483:ARG:HG3	2.03	0.41
1:A:297:SER:OG	1:A:427:LYS:O	2.26	0.41
1:C:194:LEU:HD23	1:C:194:LEU:HA	1.92	0.41
1:B:471:LYS:HD3	1:B:471:LYS:HA	1.84	0.41
1:C:91:ASN:O	1:C:94:ASP:HB2	2.21	0.41
1:D:334:PHE:HZ	1:D:371:LEU:HD21	1.86	0.41
1:C:804:LEU:HD23	1:C:818:PHE:CE2	2.56	0.40
1:D:471:LYS:HD3	1:D:471:LYS:HA	1.83	0.40
1:D:575:ARG:HA	1:D:575:ARG:HD2	1.77	0.40
1:A:859:ARG:H	1:A:859:ARG:HG3	1.63	0.40
1:C:520:ILE:O	1:C:524:PHE:HB2	2.21	0.40
1:C:540:ALA:HB2	1:C:670:THR:HB	2.02	0.40
1:A:769:ILE:CG2	1:A:770:GLU:HA	2.52	0.40
1:B:281:GLU:OE2	1:B:282:ARG:NH1	2.50	0.40
1:A:873:TRP:CE3	1:A:876:VAL:HG21	2.55	0.40
1:B:262:VAL:HG22	1:B:319:LYS:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ILE:HB	1:C:252:THR:HG23	2.03	0.40
1:C:368:LYS:HE2	1:C:368:LYS:HB3	1.84	0.40
1:C:304:TYR:CZ	1:C:457:GLU:HB2	2.56	0.40
1:D:581:SER:HB2	1:D:634:PHE:CZ	2.56	0.40
1:B:15:ILE:HD11	1:B:277:ILE:HG21	2.03	0.40
1:B:482:VAL:O	1:B:484:PRO:HD3	2.21	0.40
1:B:532:PHE:CG	1:B:533:PRO:HD2	2.57	0.40
1:B:855:ASP:HA	1:B:858:ARG:HH11	1.86	0.40
1:D:99:LYS:HD2	1:D:197:TYR:CE2	2.56	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	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

All (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
1	D	744	ALA

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Mol	Chain	Res	Type
1	A	813	VAL
1	B	765	ASP
1	D	532	PHE

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	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

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	40	LEU
1	A	57	GLN
1	A	74	VAL
1	A	91	ASN
1	A	96	ILE
1	A	309	THR
1	A	489	LEU
1	A	507	PHE
1	A	613	ASP
1	A	688	ARG
1	A	781	LEU
1	A	826	ASP
1	B	13	ASN
1	B	21	ILE
1	B	40	LEU
1	B	57	GLN
1	B	74	VAL

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Mol	Chain	Res	Type
1	B	110	ASP
1	B	215	THR
1	B	326	GLU
1	B	489	LEU
1	B	610	GLU
1	B	613	ASP
1	B	771	SER
1	B	781	LEU
1	B	804	LEU
1	C	13	ASN
1	C	21	ILE
1	C	40	LEU
1	C	74	VAL
1	C	91	ASN
1	C	227	MET
1	C	236	LEU
1	C	507	PHE
1	C	688	ARG
1	C	771	SER
1	C	781	LEU
1	C	827	GLU
1	C	881	ASP
1	C	883	LEU
1	D	21	ILE
1	D	215	THR
1	D	239	ASP
1	D	507	PHE
1	D	753	MET
1	D	781	LEU
1	D	828	LYS
1	D	859	ARG

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 ⓘ

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%)
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

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

All (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
3	D	1886	ATP	C4-C5-N7	-2.98	106.53	109.41
3	C	1886	ATP	C4-C5-N7	-2.88	106.63	109.41
3	A	1886	ATP	C4-C5-N7	-2.80	106.71	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

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	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

All (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
1	D	767	THR	5.7
1	B	146	HIS	5.7
1	D	535	SER	5.7
1	B	810	SER	5.2
1	B	744	ALA	5.2
1	D	26	THR	5.1
1	D	745	THR	4.9
1	B	768	SER	4.8
1	A	146	HIS	4.8
1	B	147	ALA	4.8
1	B	148	ASN	4.6
1	C	375	ASP	4.5
1	B	145	SER	4.5
1	C	146	HIS	4.5
1	D	810	SER	4.5
1	B	219	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	375	ASP	4.4
1	B	446	GLY	4.3
1	A	218	ARG	4.3
1	D	533	PRO	4.3
1	A	570	THR	4.2
1	A	809	LEU	4.2
1	A	859	ARG	4.2
1	D	532	PHE	4.1
1	C	745	THR	4.1
1	A	534	GLY	4.1
1	B	144	GLY	4.0
1	C	810	SER	4.0
1	C	532	PHE	3.9
1	D	219	ASP	3.8
1	A	816	GLU	3.7
1	A	145	SER	3.6
1	C	768	SER	3.6
1	A	745	THR	3.5
1	D	768	SER	3.4
1	B	26	THR	3.4
1	B	743	ALA	3.4
1	B	770	GLU	3.4
1	C	219	ASP	3.4
1	D	292	THR	3.4
1	D	493	THR	3.4
1	D	536	LYS	3.4
1	B	217	LYS	3.4
1	A	768	SER	3.4
1	D	624	LYS	3.4
1	A	219	ASP	3.3
1	A	810	SER	3.3
1	B	215	THR	3.2
1	D	570	THR	3.2
1	B	746	GLY	3.2
1	A	569	ALA	3.2
1	A	624	LYS	3.2
1	D	216	THR	3.1
1	B	218	ARG	3.1
1	C	217	LYS	3.1
1	C	569	ALA	3.0
1	A	766	PRO	3.0
1	D	218	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	807	ILE	3.0
1	B	533	PRO	3.0
1	B	858	ARG	3.0
1	D	723	ASN	3.0
1	B	374	ASP	3.0
1	D	617	ARG	2.9
1	D	822	HIS	2.9
1	A	533	PRO	2.9
1	D	531	THR	2.9
1	B	807	ILE	2.9
1	C	841	ARG	2.9
1	B	722	LYS	2.9
1	C	220	GLU	2.9
1	D	632	ASN	2.9
1	C	746	GLY	2.9
1	D	179	GLN	2.8
1	B	628	SER	2.8
1	C	533	PRO	2.8
1	C	772	GLU	2.8
1	D	840	ASP	2.8
1	B	809	LEU	2.8
1	D	770	GLU	2.8
1	D	482	VAL	2.7
1	B	808	ASP	2.7
1	C	812	PRO	2.7
1	D	29	SER	2.7
1	D	571	TYR	2.7
1	C	567	LYS	2.6
1	B	356	ASP	2.6
1	B	569	ALA	2.6
1	A	743	ALA	2.6
1	A	411	HIS	2.6
1	B	170	GLY	2.6
1	D	140	PHE	2.6
1	B	500	ALA	2.5
1	A	499	SER	2.5
1	A	345	GLN	2.5
1	A	631	SER	2.5
1	B	511	MET	2.5
1	A	744	ALA	2.5
1	C	446	GLY	2.5
1	B	772	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	747	GLU	2.5
1	C	299	PRO	2.5
1	B	87	GLN	2.5
1	D	340	LYS	2.5
1	B	92	PRO	2.4
1	C	142	GLN	2.4
1	C	744	ALA	2.4
1	B	747	GLU	2.4
1	A	808	ASP	2.4
1	A	841	ARG	2.4
1	A	374	ASP	2.4
1	D	351	GLN	2.4
1	C	855	ASP	2.4
1	A	446	GLY	2.4
1	B	748	ALA	2.4
1	D	562	GLU	2.4
1	C	218	ARG	2.4
1	D	809	LEU	2.3
1	A	772	GLU	2.3
1	D	722	LYS	2.3
1	A	220	GLU	2.3
1	B	593	GLU	2.3
1	C	593	GLU	2.3
1	C	499	SER	2.3
1	A	144	GLY	2.3
1	B	534	GLY	2.3
1	A	812	PRO	2.3
1	D	812	PRO	2.3
1	A	344	TYR	2.3
1	C	583	ALA	2.3
1	A	807	ILE	2.3
1	D	356	ASP	2.3
1	D	236	LEU	2.3
1	B	447	SER	2.3
1	A	147	ALA	2.3
1	B	443	ASN	2.3
1	B	806	GLN	2.3
1	C	411	HIS	2.3
1	D	28	ASP	2.3
1	C	147	ALA	2.3
1	C	342	LEU	2.3
1	D	534	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	844	GLN	2.3
1	B	375	ASP	2.2
1	D	841	ARG	2.2
1	A	617	ARG	2.2
1	B	841	ARG	2.2
1	C	143	ALA	2.2
1	B	236	LEU	2.2
1	B	445	LEU	2.2
1	D	631	SER	2.2
1	C	352	ARG	2.2
1	B	631	SER	2.2
1	A	765	ASP	2.1
1	C	443	ASN	2.1
1	B	420	LYS	2.1
1	B	423	LYS	2.1
1	B	749	LYS	2.1
1	D	217	LYS	2.1
1	D	348	LYS	2.1
1	B	827	GLU	2.1
1	C	570	THR	2.1
1	D	442	GLU	2.1
1	B	567	LYS	2.1
1	C	809	LEU	2.1
1	B	344	TYR	2.1
1	A	723	ASN	2.1
1	C	813	VAL	2.1
1	A	115	ASP	2.1
1	B	293	ALA	2.1
1	B	115	ASP	2.0
1	B	456	ARG	2.0
1	D	496	LYS	2.0
1	A	217	LYS	2.0
1	C	806	GLN	2.0
1	D	769	ILE	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, 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.