



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 AM GMT

PDB ID : 3B2Q  
Title : Intermediate position of ATP on its trail to the binding pocket inside the subunit B mutant R416W of the energy converter A1Ao ATP synthase  
Authors : Kumar, A.; Manimekalai, M.S.S.; Balakrishna, A.M.; Hunke, C.; Gruber, G.  
Deposited on : 2007-10-19  
Resolution : 2.10 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

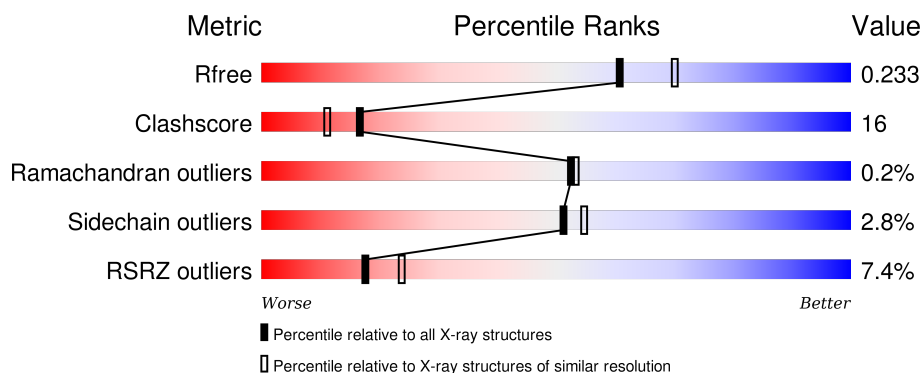
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	A	469	<div> <div>7%</div> <div>62%</div> <div>29%</div> <div>7%</div> </div>
1	B	469	<div> <div>7%</div> <div>66%</div> <div>25%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ATP	A	461	-	-	X	X
4	CIT	B	463	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7577 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 V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3366	2132	585	638	11			
1	B	431	Total	C	N	O	S	0	0	0
			3326	2109	575	631	11			

There are 22 discrepancies between the modelled and reference sequences:

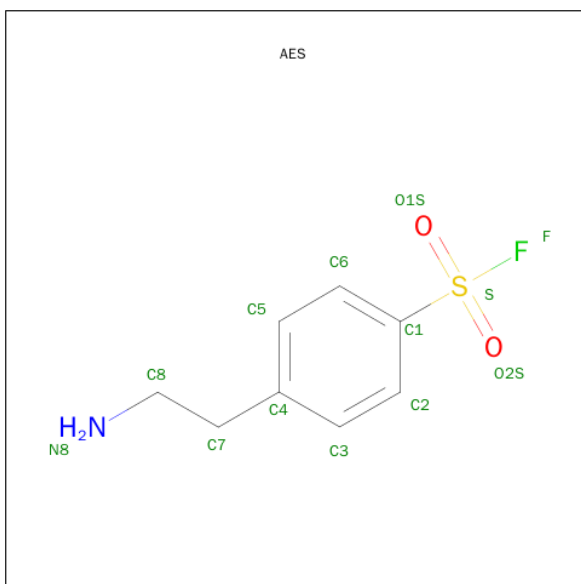
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q60187
A	-7	LYS	-	EXPRESSION TAG	UNP Q60187
A	-6	HIS	-	EXPRESSION TAG	UNP Q60187
A	-5	HIS	-	EXPRESSION TAG	UNP Q60187
A	-4	HIS	-	EXPRESSION TAG	UNP Q60187
A	-3	HIS	-	EXPRESSION TAG	UNP Q60187
A	-2	HIS	-	EXPRESSION TAG	UNP Q60187
A	-1	HIS	-	EXPRESSION TAG	UNP Q60187
A	0	PRO	-	EXPRESSION TAG	UNP Q60187
A	2	VAL	ALA	SEE REMARK 999	UNP Q60187
A	416	TRP	ARG	ENGINEERED	UNP Q60187
B	-8	MET	-	EXPRESSION TAG	UNP Q60187
B	-7	LYS	-	EXPRESSION TAG	UNP Q60187
B	-6	HIS	-	EXPRESSION TAG	UNP Q60187
B	-5	HIS	-	EXPRESSION TAG	UNP Q60187
B	-4	HIS	-	EXPRESSION TAG	UNP Q60187
B	-3	HIS	-	EXPRESSION TAG	UNP Q60187
B	-2	HIS	-	EXPRESSION TAG	UNP Q60187
B	-1	HIS	-	EXPRESSION TAG	UNP Q60187
B	0	PRO	-	EXPRESSION TAG	UNP Q60187
B	2	VAL	ALA	SEE REMARK 999	UNP Q60187
B	416	TRP	ARG	ENGINEERED	UNP Q60187

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



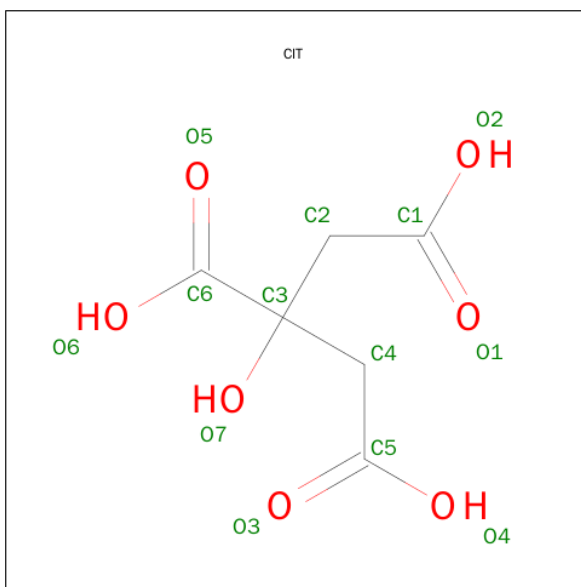
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula:  $\text{C}_8\text{H}_{10}\text{FNO}_2\text{S}$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	0	0
			13	8	1	1	2	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula:  $\text{C}_6\text{H}_8\text{O}_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			13	6	7		

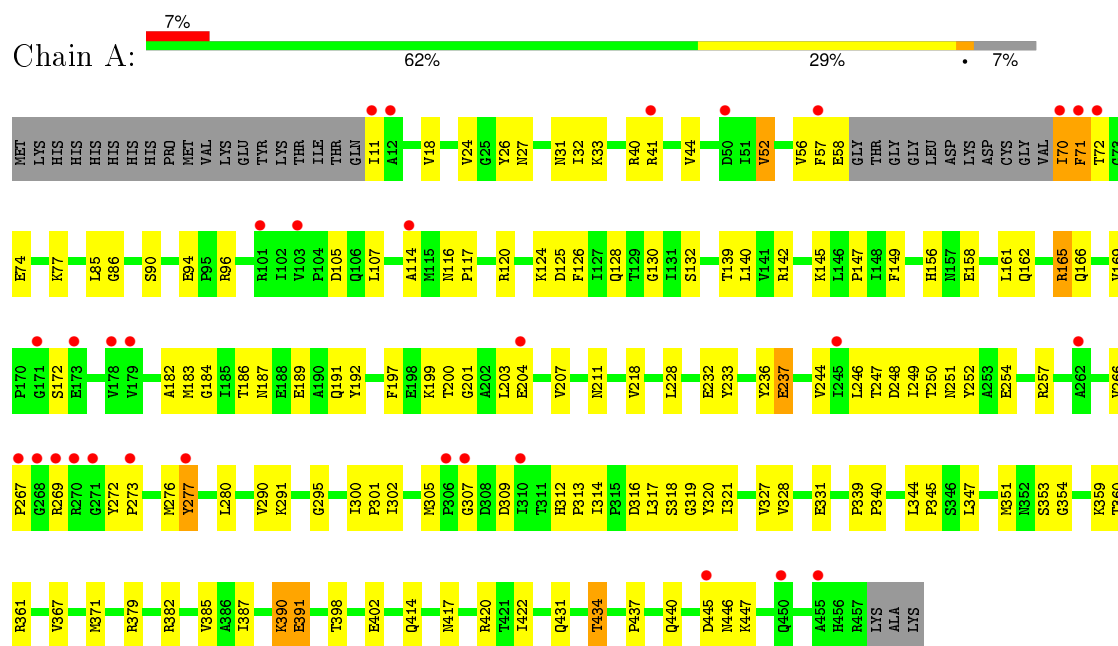
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	430	Total	O	0	0
			430	430		
5	B	398	Total	O	0	0
			398	398		

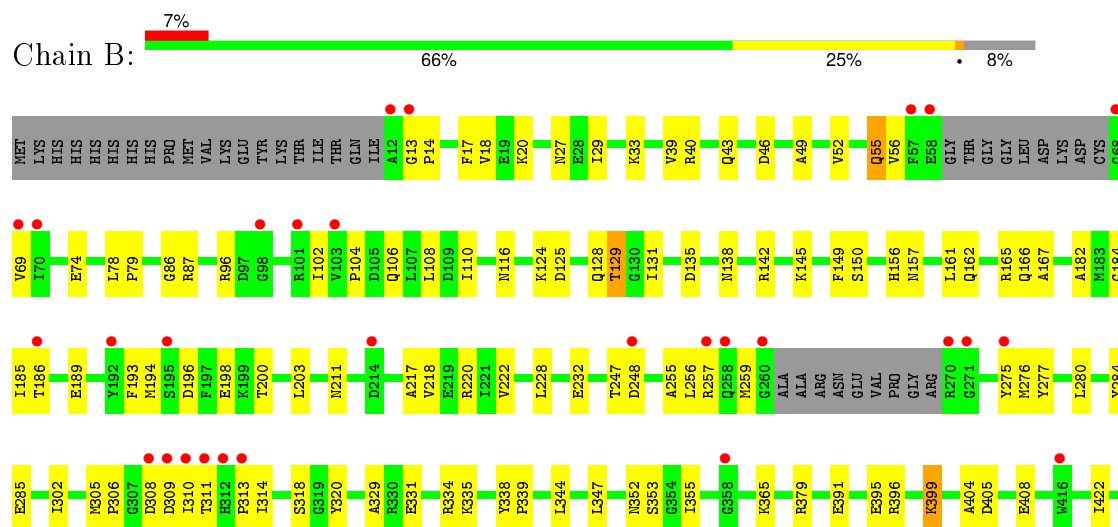
### 3 Residue-property plots [i](#)

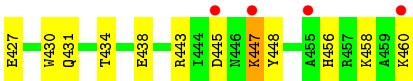
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: V-type ATP synthase beta chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.47Å 96.09Å 130.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.96 – 2.10 26.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.1 (26.96-2.10) 94.3 (26.96-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.189 , 0.237 0.186 , 0.233	Depositor DCC
$R_{free}$ test set	5504 reflections (11.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 70.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 54111 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7577	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AES, ATP, CIT

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	0.30	0/3432	0.61	0/4656
1	B	0.31	0/3390	0.61	0/4594
All	All	0.31	0/6822	0.61	0/9250

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3366	0	3367	133	0
1	B	3326	0	3331	97	0
2	A	31	0	12	9	0
3	B	13	0	10	0	0
4	B	13	0	5	0	0
5	A	430	0	0	14	0
5	B	398	0	0	9	0
All	All	7577	0	6725	222	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 16.

All (222) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LYS:HD2	1:B:447:LYS:H	1.26	0.96
1:A:70:ILE:HD13	1:A:72:THR:H	1.35	0.90
1:B:184:GLY:H	1:B:211:ASN:HD22	1.14	0.88
1:A:18:VAL:HG22	1:A:52:VAL:HG13	1.57	0.85
1:B:220:ARG:HD2	1:B:255:ALA:HB2	1.60	0.83
1:A:266:VAL:HB	1:A:269:ARG:HD2	1.59	0.82
1:B:129:THR:HG23	1:B:131:ILE:H	1.44	0.80
1:A:339:PRO:HG2	5:A:680:HOH:O	1.85	0.77
1:B:458:LYS:HB2	1:B:460:LYS:HE3	1.67	0.76
1:B:447:LYS:CD	1:B:447:LYS:H	1.99	0.74
1:A:120:ARG:HD2	5:B:1282:HOH:O	1.87	0.74
1:B:162:GLN:HE21	1:B:166:GLN:HE22	1.36	0.73
1:A:70:ILE:HG21	5:A:687:HOH:O	1.87	0.73
1:A:184:GLY:H	1:A:211:ASN:HD22	1.37	0.70
1:B:129:THR:HG22	1:B:135:ASP:OD1	1.91	0.69
1:A:321:ILE:HD12	2:A:461:ATP:N7	2.07	0.69
1:A:132:SER:H	1:A:414:GLN:HE22	1.41	0.69
1:A:321:ILE:CD1	2:A:461:ATP:N7	2.56	0.69
1:A:165:ARG:HH12	1:A:417:ASN:ND2	1.91	0.69
1:B:186:THR:OG1	1:B:189:GLU:HG3	1.92	0.68
1:A:18:VAL:HG22	1:A:52:VAL:CG1	2.24	0.68
1:B:129:THR:CG2	1:B:131:ILE:H	2.08	0.66
1:B:308:ASP:OD2	1:B:310:ILE:HG12	1.96	0.66
1:A:70:ILE:HD13	1:A:72:THR:N	2.08	0.66
1:A:313:PRO:HG2	5:A:602:HOH:O	1.95	0.65
1:A:169:VAL:HG22	1:A:172:SER:HB2	1.78	0.65
1:B:157:ASN:O	1:B:161:LEU:HD23	1.96	0.65
1:A:24:VAL:HG21	1:A:44:VAL:HG21	1.77	0.65
1:B:310:ILE:HG13	1:B:311:THR:N	2.09	0.64
1:A:273:PRO:HG2	1:A:276:MET:CG	2.27	0.64
1:B:344:LEU:HD11	1:B:379:ARG:HD3	1.80	0.64
1:B:391:GLU:HG2	5:B:1186:HOH:O	1.98	0.63
1:A:277:TYR:OH	1:B:334:ARG:NH1	2.32	0.62
1:B:259:MET:HA	1:B:259:MET:HE3	1.80	0.62
1:A:31:ASN:OD1	1:A:41:ARG:HD2	1.99	0.62
1:B:162:GLN:HE21	1:B:166:GLN:NE2	1.97	0.62
1:B:184:GLY:H	1:B:211:ASN:ND2	1.92	0.61
1:A:70:ILE:CD1	1:A:72:THR:H	2.11	0.61
1:B:458:LYS:O	1:B:460:LYS:HG2	2.01	0.61
1:B:344:LEU:CD1	1:B:379:ARG:HD3	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLN:HA	1:A:165:ARG:HD3	1.83	0.60
1:B:257:ARG:HG2	1:B:257:ARG:HH11	1.64	0.60
1:B:13:GLY:HA2	1:B:55:GLN:HG2	1.83	0.60
1:A:244:VAL:HG12	1:A:246:LEU:HD11	1.84	0.60
1:A:24:VAL:CG2	1:A:44:VAL:HG21	2.32	0.59
1:A:273:PRO:HG2	1:A:276:MET:HG2	1.83	0.59
1:A:398:THR:O	1:A:402:GLU:HG3	2.01	0.59
1:A:390:LYS:H	1:A:390:LYS:HE3	1.68	0.58
1:A:280:LEU:HD11	1:A:317:LEU:HD23	1.86	0.57
1:A:244:VAL:HG12	1:A:246:LEU:CD1	2.35	0.57
1:B:306:PRO:HD2	1:B:314:ILE:HG12	1.85	0.57
2:A:461:ATP:N3	1:B:149:PHE:CE2	2.73	0.56
1:A:347:LEU:HD22	1:B:347:LEU:HD22	1.87	0.56
1:A:145:LYS:HD2	5:A:513:HOH:O	2.05	0.56
1:B:352:ASN:OD1	1:B:365:LYS:HE3	2.05	0.56
1:B:228:LEU:O	1:B:232:GLU:HG3	2.05	0.56
1:A:236:TYR:HE1	1:A:291:LYS:HB2	1.71	0.56
1:A:124:LYS:HA	1:A:353:SER:HB3	1.88	0.55
1:B:14:PRO:HG2	1:B:56:VAL:HG22	1.89	0.55
1:B:257:ARG:HG2	1:B:257:ARG:NH1	2.22	0.55
1:B:447:LYS:HG3	5:B:1173:HOH:O	2.05	0.55
1:B:313:PRO:HB3	5:B:1102:HOH:O	2.06	0.55
1:A:236:TYR:CE1	1:A:291:LYS:HB2	2.43	0.54
1:A:142:ARG:NH2	1:A:169:VAL:HG23	2.23	0.54
1:B:276:MET:O	1:B:280:LEU:HD23	2.08	0.53
1:A:187:ASN:O	1:A:191:GLN:HG2	2.08	0.53
1:A:316:ASP:OD2	1:B:329:ALA:HB1	2.09	0.53
1:A:249:ILE:O	1:A:252:TYR:HB3	2.09	0.53
1:B:106:GLN:OE1	1:B:108:LEU:HD21	2.09	0.53
1:A:390:LYS:H	1:A:390:LYS:CE	2.22	0.53
1:B:165:ARG:HD3	1:B:196:ASP:OD1	2.08	0.53
1:B:194:MET:O	1:B:198:GLU:HG3	2.09	0.53
1:A:319:GLY:HA2	5:A:552:HOH:O	2.09	0.52
1:A:142:ARG:CZ	1:A:169:VAL:HG23	2.39	0.52
1:A:344:LEU:CD1	1:A:379:ARG:HD3	2.39	0.52
1:B:69:VAL:HG22	1:B:69:VAL:O	2.09	0.52
1:A:344:LEU:HD11	1:A:379:ARG:HD3	1.92	0.52
1:A:116:ASN:N	1:A:117:PRO:HD3	2.25	0.51
1:B:399:LYS:HE2	1:B:399:LYS:HA	1.91	0.51
1:B:128:GLN:NE2	1:B:422:ILE:H	2.07	0.51
1:A:183:MET:N	1:A:247:THR:O	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:HD2	1:A:314:ILE:HG22	1.93	0.51
1:A:33:LYS:HB3	1:A:74:GLU:HG2	1.93	0.50
2:A:461:ATP:C2	1:B:149:PHE:HE2	2.30	0.50
1:A:162:GLN:HE21	1:A:166:GLN:HE22	1.59	0.50
1:A:250:THR:O	1:A:254:GLU:HG2	2.11	0.50
1:B:29:ILE:HD13	1:B:43:GLN:HG3	1.92	0.50
1:B:27:ASN:HA	1:B:43:GLN:HG2	1.93	0.50
1:A:331:GLU:HG3	1:B:277:TYR:CG	2.47	0.50
1:A:142:ARG:CZ	1:A:169:VAL:CG2	2.90	0.49
1:B:405:ASP:HB3	5:B:1213:HOH:O	2.10	0.49
1:B:124:LYS:HA	1:B:353:SER:HB3	1.94	0.49
1:A:248:ASP:OD2	1:A:302:ILE:O	2.29	0.49
1:B:125:ASP:HB2	1:B:142:ARG:HD2	1.94	0.49
1:A:305:MET:CE	1:A:305:MET:HA	2.42	0.49
1:A:321:ILE:HD13	2:A:461:ATP:N7	2.26	0.49
1:B:310:ILE:HG13	1:B:311:THR:H	1.74	0.49
1:A:233:TYR:O	1:A:237:GLU:HB2	2.12	0.49
1:A:31:ASN:O	1:A:32:ILE:HD13	2.13	0.49
1:A:244:VAL:CG1	1:A:246:LEU:HD11	2.43	0.49
1:A:445:ASP:OD1	1:A:447:LYS:HD3	2.13	0.49
1:B:18:VAL:HG13	1:B:74:GLU:O	2.11	0.49
1:A:199:LYS:HG3	1:A:200:THR:N	2.26	0.49
1:A:70:ILE:HD13	1:A:70:ILE:C	2.33	0.48
1:A:437:PRO:HB2	1:A:440:GLN:HG2	1.96	0.48
1:A:125:ASP:HB2	1:A:142:ARG:HD2	1.94	0.48
1:B:129:THR:HG23	1:B:131:ILE:N	2.20	0.48
1:A:116:ASN:N	1:A:117:PRO:CD	2.76	0.48
1:A:273:PRO:O	1:A:276:MET:HB2	2.14	0.48
1:A:248:ASP:OD2	1:A:248:ASP:C	2.52	0.48
1:B:33:LYS:HA	1:B:39:VAL:HG12	1.95	0.48
1:A:162:GLN:O	1:A:166:GLN:HG3	2.14	0.47
5:A:554:HOH:O	1:B:285:GLU:HG2	2.13	0.47
1:B:102:ILE:O	1:B:104:PRO:HD3	2.13	0.47
1:A:445:ASP:OD2	1:A:446:ASN:N	2.47	0.47
1:A:26:TYR:O	1:A:27:ASN:HB2	2.14	0.47
1:A:11:ILE:HB	1:A:58:GLU:H	1.78	0.47
1:A:318:SER:HA	2:A:461:ATP:HN61	1.79	0.47
1:A:147:PRO:HB3	1:A:301:PRO:HG2	1.96	0.46
1:A:182:ALA:HA	1:A:247:THR:O	2.15	0.46
1:B:20:LYS:HD2	1:B:49:ALA:O	2.15	0.46
1:A:156:HIS:HE1	5:A:672:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASP:OD2	1:B:259:MET:O	2.33	0.46
1:A:86:GLY:HA2	1:A:203:LEU:O	2.15	0.46
1:A:139:THR:HB	1:A:351:MET:HG3	1.97	0.46
1:A:70:ILE:O	1:A:71:PHE:C	2.52	0.46
1:B:218:VAL:HG23	5:B:1113:HOH:O	2.15	0.46
1:B:438:GLU:CD	1:B:456:HIS:HE2	2.19	0.46
1:A:162:GLN:HE21	1:A:166:GLN:NE2	2.14	0.46
1:A:169:VAL:HG22	1:A:172:SER:CB	2.45	0.46
1:A:149:PHE:CE1	1:A:305:MET:HG2	2.51	0.46
1:A:218:VAL:HG23	5:A:481:HOH:O	2.16	0.46
1:B:275:TYR:HB2	5:B:1078:HOH:O	2.15	0.46
1:B:311:THR:O	1:B:313:PRO:HD3	2.16	0.45
1:B:302:ILE:HD12	1:B:302:ILE:N	2.31	0.45
1:A:169:VAL:HG13	1:A:169:VAL:O	2.17	0.45
1:B:161:LEU:HD21	1:B:193:PHE:CE2	2.52	0.45
1:B:20:LYS:NZ	1:B:52:VAL:HG22	2.31	0.45
1:A:186:THR:HG23	1:A:189:GLU:OE2	2.15	0.45
2:A:461:ATP:C2	1:B:149:PHE:CE2	3.04	0.45
1:A:382:ARG:O	1:A:385:VAL:HG12	2.17	0.45
1:A:367:VAL:O	1:A:371:MET:HG3	2.16	0.45
1:A:280:LEU:CD1	1:A:317:LEU:HD23	2.47	0.45
1:A:11:ILE:HG21	1:A:58:GLU:HA	1.98	0.45
1:B:247:THR:HA	1:B:248:ASP:HA	1.52	0.45
1:A:248:ASP:O	1:A:249:ILE:C	2.55	0.45
1:B:256:LEU:O	1:B:257:ARG:C	2.55	0.45
1:A:189:GLU:O	1:A:192:TYR:HB3	2.16	0.44
1:A:126:PHE:HB2	1:A:354:GLY:O	2.17	0.44
1:B:14:PRO:HG2	1:B:56:VAL:CG2	2.47	0.44
1:A:353:SER:O	1:A:359:LYS:NZ	2.31	0.44
1:B:438:GLU:OE2	1:B:456:HIS:NE2	2.51	0.44
1:B:247:THR:HG23	1:B:247:THR:O	2.17	0.44
1:B:310:ILE:HG13	1:B:311:THR:HG23	1.99	0.44
1:A:290:VAL:HG22	1:A:295:GLY:O	2.18	0.44
1:A:431:GLN:O	1:A:434:THR:HB	2.17	0.44
1:B:150:SER:OG	1:B:156:HIS:HD2	2.00	0.44
1:A:267:PRO:HG3	1:A:272:TYR:CE1	2.52	0.44
1:B:33:LYS:NZ	1:B:33:LYS:HB3	2.33	0.44
1:A:90:SER:HA	1:A:96:ARG:HE	1.83	0.44
1:A:70:ILE:N	5:A:526:HOH:O	2.50	0.44
1:A:40:ARG:HD2	1:A:56:VAL:HG11	2.00	0.44
1:B:445:ASP:OD2	1:B:448:TYR:CD1	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LYS:HD3	5:A:855:HOH:O	2.18	0.43
1:A:85:LEU:HD23	1:A:207:VAL:CG2	2.48	0.43
1:B:78:LEU:HD12	1:B:79:PRO:HD2	2.01	0.43
1:A:331:GLU:HG3	1:B:277:TYR:CD2	2.54	0.43
1:A:445:ASP:CG	1:A:447:LYS:HG2	2.38	0.43
1:B:331:GLU:HG2	1:B:335:LYS:HE2	1.99	0.43
1:A:327:VAL:CG1	2:A:461:ATP:O2A	2.67	0.43
1:A:130:GLY:HA2	1:A:420:ARG:O	2.19	0.43
1:A:328:VAL:HG13	1:A:340:PRO:HG2	2.01	0.43
1:A:162:GLN:HA	1:A:165:ARG:CD	2.49	0.43
1:A:312:HIS:HE1	5:A:615:HOH:O	2.02	0.43
1:A:70:ILE:HD13	1:A:71:PHE:N	2.33	0.43
1:A:158:GLU:OE1	1:A:158:GLU:N	2.47	0.43
1:A:307:GLY:HA2	1:B:309:ASP:OD1	2.18	0.43
1:B:87:ARG:HG3	1:B:102:ILE:HD11	2.00	0.43
1:B:404:ALA:O	1:B:408:GLU:HG3	2.20	0.42
1:B:165:ARG:CD	1:B:200:THR:HG21	2.49	0.42
1:B:110:ILE:HD12	1:B:110:ILE:C	2.40	0.42
1:B:165:ARG:HD2	1:B:200:THR:HG21	2.02	0.42
1:B:86:GLY:HA2	1:B:203:LEU:O	2.20	0.42
1:A:249:ILE:O	1:A:252:TYR:N	2.53	0.42
1:B:20:LYS:HZ3	1:B:52:VAL:HG22	1.85	0.42
1:A:90:SER:OG	1:A:94:GLU:HG2	2.19	0.42
1:A:228:LEU:O	1:A:232:GLU:HG3	2.19	0.42
1:A:360:THR:OG1	1:A:361:ARG:N	2.52	0.42
1:A:201:GLY:O	1:A:204:GLU:HG2	2.19	0.42
1:A:345:PRO:HG3	1:B:318:SER:HB2	2.02	0.42
1:A:128:GLN:NE2	1:A:422:ILE:H	2.18	0.41
1:B:217:ALA:HB2	5:B:1180:HOH:O	2.19	0.41
1:A:142:ARG:NH2	1:A:169:VAL:CG2	2.83	0.41
1:B:338:TYR:CD1	1:B:339:PRO:HA	2.55	0.41
1:A:161:LEU:O	1:A:165:ARG:HD2	2.21	0.41
1:B:145:LYS:HD3	1:B:284:TYR:O	2.21	0.41
1:A:140:LEU:HD22	1:A:300:ILE:HD11	2.03	0.41
1:A:165:ARG:NH2	1:A:200:THR:HG21	2.35	0.41
1:B:128:GLN:O	1:B:167:ALA:HA	2.20	0.41
1:B:396:ARG:HD3	1:B:396:ARG:C	2.41	0.41
1:B:430:TRP:O	1:B:434:THR:HG23	2.21	0.41
1:B:182:ALA:HB1	1:B:185:ILE:HG21	2.01	0.41
1:B:355:ILE:HD11	1:B:365:LYS:HE2	2.02	0.41
1:A:248:ASP:O	1:A:251:ASN:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:HG12	1:A:57:PHE:N	2.36	0.41
1:A:56:VAL:HG12	1:A:57:PHE:O	2.21	0.41
1:A:86:GLY:HA2	1:A:203:LEU:HG	2.03	0.41
1:B:427:GLU:O	1:B:431:GLN:HG2	2.20	0.41
1:A:191:GLN:NE2	5:A:722:HOH:O	2.53	0.41
1:A:233:TYR:CE1	1:A:237:GLU:HG2	2.56	0.41
1:B:17:PHE:CD1	1:B:222:VAL:HG12	2.56	0.40
1:A:77:LYS:HD2	1:A:107:LEU:HB3	2.04	0.40
1:B:443:ARG:NH2	5:B:1042:HOH:O	2.47	0.40
1:A:120:ARG:HA	1:A:120:ARG:HD3	1.83	0.40
1:A:273:PRO:HG2	1:A:276:MET:HG3	2.02	0.40
1:A:277:TYR:HB2	5:A:814:HOH:O	2.21	0.40
1:A:11:ILE:O	1:A:57:PHE:HA	2.22	0.40
1:A:387:ILE:O	1:B:40:ARG:NH2	2.55	0.40
1:A:197:PHE:HA	5:A:702:HOH:O	2.20	0.40
1:A:327:VAL:HG13	2:A:461:ATP:O2A	2.21	0.40
1:B:305:MET:HA	1:B:306:PRO:HD3	1.90	0.40
1:A:391:GLU:OE1	1:A:391:GLU:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/469 (92%)	418 (97%)	12 (3%)	2 (0%)	34	30
1	B	425/469 (91%)	405 (95%)	20 (5%)	0	100	100
All	All	857/938 (91%)	823 (96%)	32 (4%)	2 (0%)	52	53

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	A	114	ALA
1	A	71	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	356/384 (93%)	345 (97%)	11 (3%)	47	50
1	B	352/384 (92%)	343 (97%)	9 (3%)	54	58
All	All	708/768 (92%)	688 (97%)	20 (3%)	51	55

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	70	ILE
1	A	105	ASP
1	A	165	ARG
1	A	237	GLU
1	A	277	TYR
1	A	309	ASP
1	A	320	TYR
1	A	390	LYS
1	A	391	GLU
1	A	434	THR
1	B	55	GLN
1	B	96	ARG
1	B	116	ASN
1	B	129	THR
1	B	138	ASN
1	B	320	TYR
1	B	395	GLU
1	B	399	LYS
1	B	447	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	128	GLN
1	A	138	ASN
1	A	156	HIS
1	A	166	GLN
1	A	191	GLN
1	A	211	ASN
1	A	299	GLN
1	A	312	HIS
1	A	414	GLN
1	A	417	ASN
1	B	27	ASN
1	B	31	ASN
1	B	43	GLN
1	B	116	ASN
1	B	128	GLN
1	B	156	HIS
1	B	166	GLN
1	B	211	ASN
1	B	299	GLN
1	B	417	ASN
1	B	450	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](#)

3 ligands are modelled in this entry.

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	A	461	-	24,33,33	0.98	1 (4%)	31,52,52	2.00	5 (16%)
3	AES	B	462	-	11,13,13	1.49	1 (9%)	17,18,18	8.78	5 (29%)
4	CIT	B	463	-	3,12,12	0.97	0	3,17,17	0.44	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	A	461	-	-	0/18/38/38	0/3/3/3
3	AES	B	462	-	-	0/9/9/9	0/1/1/1
4	CIT	B	463	-	-	0/6/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	462	AES	C6-C1	2.64	1.43	1.38
2	A	461	ATP	C5-C4	3.13	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	462	AES	O2S-S-C1	-30.48	77.75	110.73
3	B	462	AES	F-S-O2S	-13.67	74.12	106.52
2	A	461	ATP	N3-C2-N1	-6.69	123.77	128.89
3	B	462	AES	O2S-S-O1S	-5.04	102.95	118.95
2	A	461	ATP	PA-O3A-PB	-4.35	120.50	132.73
2	A	461	ATP	PB-O3B-PG	-3.63	120.51	132.67
2	A	461	ATP	C4-C5-N7	-3.16	106.57	109.48
2	A	461	ATP	C2'-C1'-N9	-3.15	109.49	114.29
3	B	462	AES	F-S-O1S	2.42	112.25	106.52
3	B	462	AES	F-S-C1	12.63	131.53	102.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	461	ATP	9	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	A	436/469 (92%)	0.20	31 (7%) 19 26	12, 26, 49, 66	0
1	B	431/469 (91%)	0.13	33 (7%) 16 22	11, 24, 48, 66	0
All	All	867/938 (92%)	0.16	64 (7%) 17 24	11, 25, 49, 66	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	ILE	8.9
1	A	70	ILE	8.7
1	B	68	GLY	7.8
1	A	270	ARG	6.0
1	B	69	VAL	5.4
1	A	71	PHE	5.4
1	B	310	ILE	4.9
1	A	277	TYR	4.8
1	B	260	GLY	4.8
1	B	270	ARG	4.6
1	B	312	HIS	4.3
1	B	214	ASP	4.3
1	A	72	THR	4.2
1	B	311	THR	4.2
1	A	12	ALA	4.1
1	A	269	ARG	3.7
1	A	307	GLY	3.6
1	B	258	GLN	3.5
1	B	70	ILE	3.4
1	B	309	ASP	3.3
1	A	171	GLY	3.3
1	B	416	TRP	3.3
1	B	460	LYS	3.2
1	A	173	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	101	ARG	3.1
1	B	58	GLU	3.0
1	B	57	PHE	3.0
1	A	50	ASP	2.9
1	A	57	PHE	2.9
1	B	271	GLY	2.8
1	A	306	PRO	2.8
1	B	248	ASP	2.8
1	A	268	GLY	2.8
1	A	103	VAL	2.7
1	B	447	LYS	2.5
1	A	455	ALA	2.5
1	B	186	THR	2.5
1	A	450	GLN	2.5
1	B	455	ALA	2.4
1	B	313	PRO	2.4
1	A	262	ALA	2.4
1	A	179	VAL	2.4
1	B	12	ALA	2.4
1	A	267	PRO	2.4
1	B	195	SER	2.4
1	B	103	VAL	2.3
1	A	310	ILE	2.3
1	A	41	ARG	2.3
1	B	98	GLY	2.3
1	A	101	ARG	2.3
1	A	245	ILE	2.3
1	B	13	GLY	2.3
1	A	204	GLU	2.2
1	B	308	ASP	2.2
1	B	275	TYR	2.1
1	A	178	VAL	2.1
1	A	273	PRO	2.1
1	B	257	ARG	2.1
1	A	271	GLY	2.1
1	A	445	ASP	2.1
1	B	445	ASP	2.1
1	A	114	ALA	2.0
1	B	192	TYR	2.0
1	B	358	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<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
4	CIT	B	463	13/13	0.55	0.41	13.04	68,74,75,75	0
2	ATP	A	461	31/31	0.59	0.50	10.38	44,55,71,72	0
3	AES	B	462	13/13	0.91	0.16	1.54	37,41,47,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.