



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:06 AM GMT

PDB ID : 2VYP
Title : RABBIT-MUSCLE G-ACTIN IN COMPLEX WITH MYXOBACTERIAL RHIZOPODIN
Authors : Hagelueken, G.; Albrecht, S.C.; Steinmetz, H.; Jansen, R.; Heinz, D.W.; Kalesse, M.; Schubert, W.-D.
Deposited on : 2008-07-25
Resolution : 2.35 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 (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

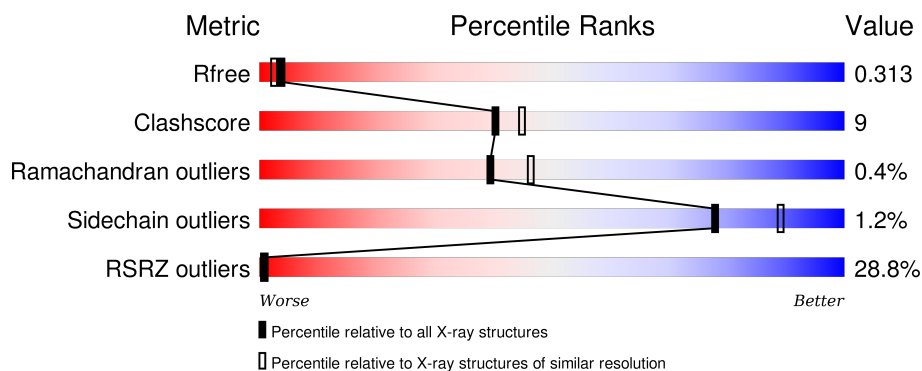
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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	377	
1	B	377	

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
5	HEZ	A	1380	-	-	-	X

2 Entry composition [i](#)

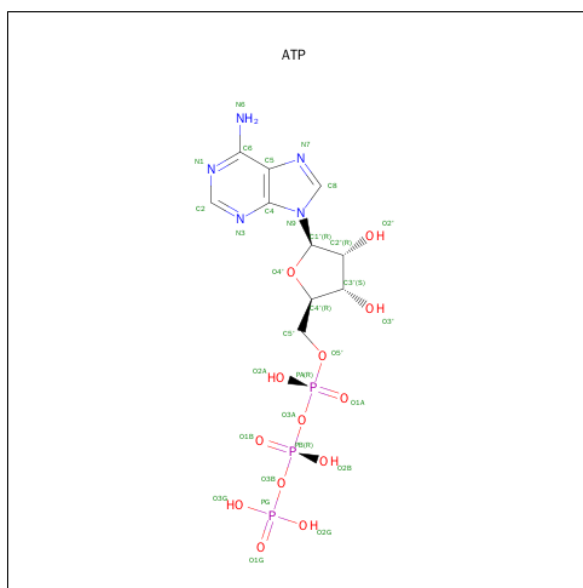
There are 6 unique types of molecules in this entry. The entry contains 5844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACTIN, ALPHA SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	4	0
			2823	1790	472	541	20			
1	B	330	Total	C	N	O	S	0	5	1
			2613	1664	432	496	21			

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

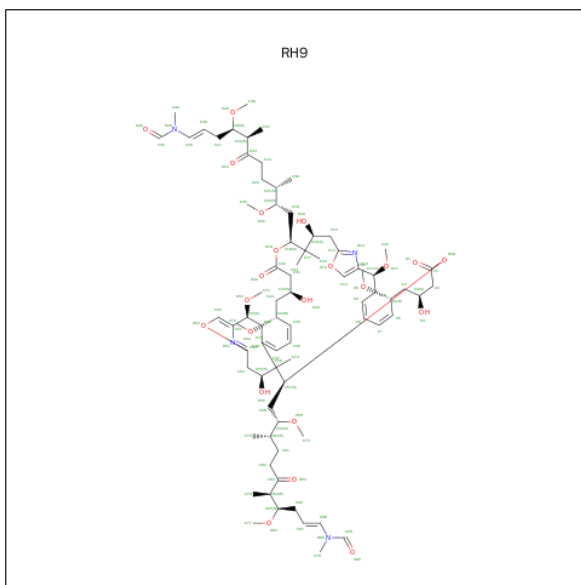


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

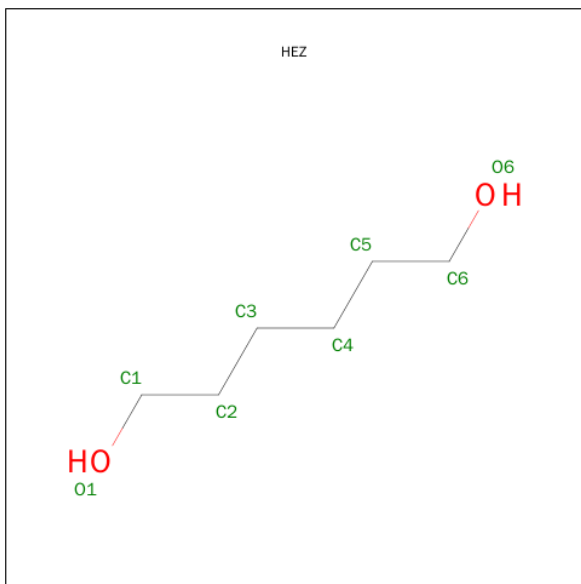
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is RHIZOPODIN (three-letter code: RH9) (formula: $C_{78}H_{124}N_4O_{22}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			104	78	4	22		

- Molecule 5 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

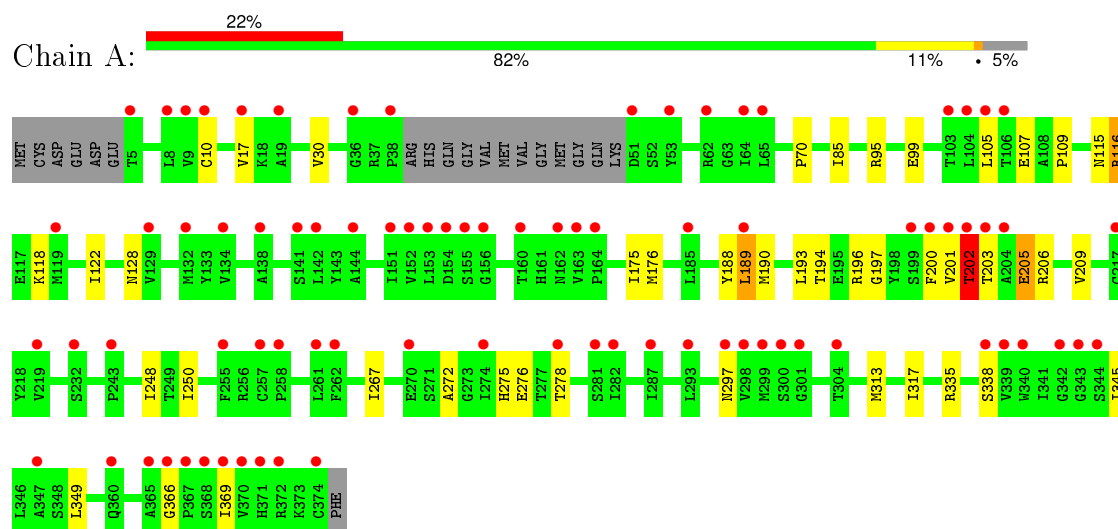
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total	O	0	0
			152	152		
6	B	62	Total	O	0	0
			62	62		

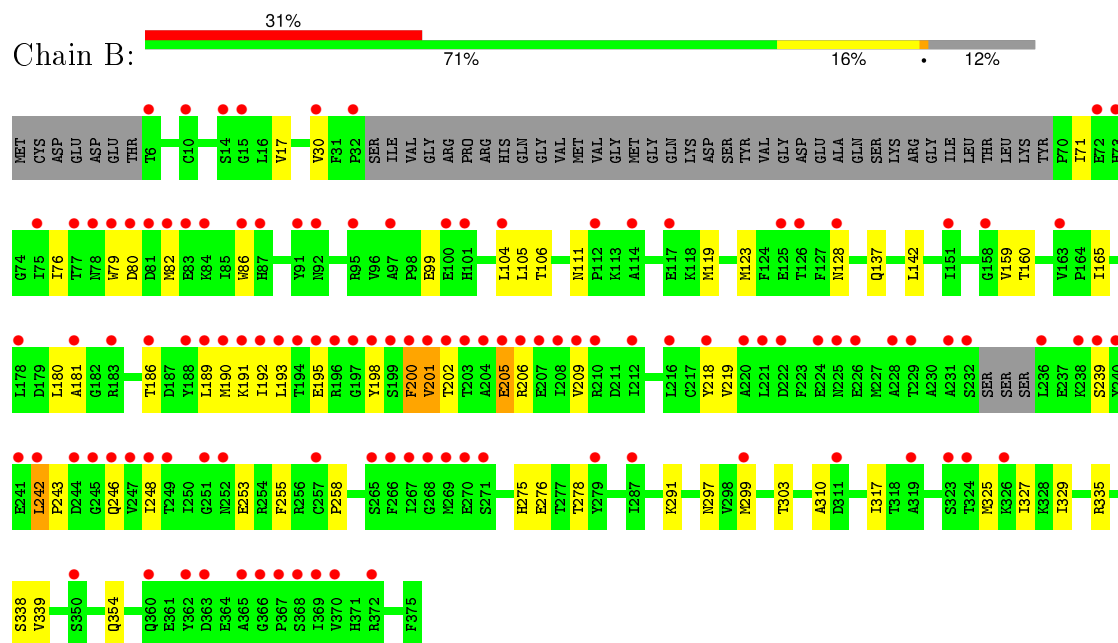
3 Residue-property plots

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 ($RSRZ > 2$). 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: ACTIN, ALPHA SKELETAL MUSCLE



• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.65Å 194.86Å 53.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.41 – 2.35 19.41 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.41-2.35) 100.0 (19.41-2.35)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.186 , 0.241 0.275 , 0.313	Depositor DCC
R_{free} test set	1759 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 34349 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5844	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: RH9, CA, HEZ, 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	0.86	0/2892	0.83	1/3920 (0.0%)
1	B	0.76	1/2685 (0.0%)	0.75	1/3637 (0.0%)
All	All	0.81	1/5577 (0.0%)	0.79	2/7557 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	80	ASP	C-O	13.96	1.49	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	ARG	CG-CD-NE	-5.62	100.00	111.80
1	B	242	LEU	N-CA-C	5.48	125.80	111.00

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	2823	0	2801	34	0
1	B	2613	0	2588	63	0
2	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	0	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	104	0	124	2	0
5	A	24	0	42	1	0
6	A	152	0	0	1	0
6	B	62	0	0	1	0
All	All	5844	0	5579	98	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 9.

All (98) 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:206:ARG:O	1:B:209:VAL:HG22	1.69	0.93
1:B:190:MET:HE2	1:B:209:VAL:HG21	1.48	0.92
1:B:242:LEU:HD21	1:B:248:ILE:CD1	2.02	0.89
1:A:107:GLU:OE1	1:A:116:ARG:HD2	1.86	0.76
1:B:200:PHE:O	1:B:202:THR:HG22	1.85	0.75
1:A:193:LEU:HD21	1:A:250:ILE:HG21	1.69	0.73
1:B:189:LEU:HD12	1:B:192:ILE:HD11	1.69	0.73
1:B:190:MET:HE2	1:B:209:VAL:CG2	2.20	0.71
1:A:70:PRO:HG2	1:A:85:ILE:HD12	1.71	0.70
1:A:95[B]:ARG:NH1	6:A:2025:HOH:O	2.25	0.69
1:A:278:THR:HG21	1:A:297:ASN:HD21	1.58	0.68
1:A:201:VAL:N	1:A:205:GLU:HG3	2.12	0.65
1:B:104:LEU:HD23	1:B:104:LEU:C	2.17	0.64
1:A:193:LEU:HD21	1:A:250:ILE:CG2	2.27	0.64
1:B:291:LYS:HG2	1:B:325:MET:SD	2.39	0.63
1:B:278:THR:HG21	1:B:297:ASN:HD21	1.63	0.63
1:B:111:ASN:HD21	1:B:119[B]:MET:HE1	1.63	0.63
1:B:190:MET:CE	1:B:206:ARG:HB2	2.29	0.62
1:B:242:LEU:HD21	1:B:248:ILE:HD12	1.81	0.62
1:A:202:THR:HG22	1:A:203:THR:H	1.65	0.61
1:B:99[B]:GLU:HG3	1:B:128:ASN:HB3	1.83	0.61
1:B:198:TYR:CZ	1:B:248:ILE:HG23	2.36	0.61
1:B:206:ARG:O	1:B:209:VAL:CG2	2.47	0.60
1:B:202:THR:HG23	1:B:205:GLU:HB2	1.81	0.60
1:B:299[A]:MET:HE1	1:B:310:ALA:HA	1.84	0.60
1:B:190:MET:HE1	1:B:206:ARG:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD13	1:B:119[A]:MET:HE1	1.84	0.59
1:B:105:LEU:HD13	1:B:119[A]:MET:CE	2.33	0.58
1:B:278:THR:CG2	1:B:297:ASN:HD21	2.15	0.58
1:A:313:MET:HE3	1:A:317:ILE:HG12	1.85	0.58
1:A:272:ALA:HB1	1:A:276:GLU:HB2	1.87	0.57
1:A:196:ARG:N	1:A:197:GLY:HA2	2.21	0.56
1:A:202:THR:HG22	1:A:203:THR:N	2.21	0.56
1:B:242:LEU:HD21	1:B:248:ILE:HD11	1.86	0.55
1:B:202:THR:HG23	1:B:205:GLU:CB	2.36	0.55
1:B:105:LEU:HD11	1:B:123:MET:HG3	1.88	0.54
1:A:349:LEU:HD22	5:A:1378:HEZ:H22	1.90	0.54
1:A:366:GLY:O	1:A:369:ILE:HG22	2.09	0.52
1:B:242:LEU:HD23	1:B:246:GLN:O	2.09	0.52
1:A:313:MET:HE3	1:A:317:ILE:CG1	2.40	0.52
1:B:190:MET:CE	1:B:209:VAL:HG21	2.32	0.52
1:B:142:LEU:HD22	1:B:165:ILE:HB	1.92	0.51
1:B:335:ARG:HA	1:B:338:SER:OG	2.10	0.51
1:B:219:VAL:HG22	1:B:258:PRO:HB2	1.92	0.51
1:B:71:ILE:HG13	1:B:82:MET:HE1	1.92	0.50
1:B:186:THR:HG23	1:B:209:VAL:HG23	1.93	0.50
1:A:190:MET:O	1:A:194:THR:HG23	2.12	0.49
1:B:303:THR:HG22	1:B:303:THR:O	2.12	0.49
1:B:106:THR:HB	1:B:137:GLN:HG3	1.94	0.48
1:B:86:TRP:CD2	1:B:123:MET:HE1	2.49	0.48
1:B:191:LYS:O	1:B:195:GLU:N	2.40	0.48
1:A:118:LYS:HE3	1:A:122:ILE:HD11	1.96	0.48
1:B:189:LEU:HD12	1:B:193:LEU:HD13	1.96	0.48
1:B:17:VAL:O	1:B:30:VAL:HA	2.14	0.47
1:A:201:VAL:HG13	1:A:202:THR:H	1.80	0.47
1:A:107:GLU:CD	1:A:116:ARG:HD2	2.35	0.47
1:A:99[B]:GLU:HG3	1:A:128:ASN:HB3	1.97	0.47
1:B:190:MET:HE2	1:B:206:ARG:HB2	1.96	0.46
1:A:70:PRO:HG2	1:A:85:ILE:CD1	2.42	0.46
1:B:190:MET:HE1	1:B:206:ARG:CB	2.45	0.46
1:B:299[A]:MET:CE	1:B:329:ILE:HG21	2.46	0.46
1:A:109:PRO:HB3	1:A:175:ILE:HD13	1.97	0.46
1:B:200:PHE:O	1:B:201:VAL:C	2.53	0.46
1:B:189:LEU:CD1	1:B:192:ILE:HD11	2.43	0.46
1:B:76:ILE:HD12	1:B:119[B]:MET:HE3	1.97	0.46
1:A:188:TYR:CD1	1:A:267:ILE:HG22	2.52	0.45
1:A:275:HIS:CD2	1:A:275:HIS:H	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:LEU:HD23	1:B:181:ALA:N	2.32	0.44
1:A:189:LEU:HD22	1:A:193:LEU:CD1	2.46	0.44
1:A:345:ILE:HD13	4:A:1377:RH9:H2C2	2.00	0.44
1:A:10:CYS:HB3	1:A:105:LEU:HD23	2.00	0.44
1:B:137:GLN:HG2	1:B:339:VAL:HG11	1.99	0.44
1:B:317:ILE:HG22	1:B:327:ILE:HD12	2.00	0.44
1:A:205:GLU:O	1:A:209:VAL:HG23	2.18	0.43
1:B:239:SER:HA	1:B:248:ILE:O	2.18	0.43
1:B:198:TYR:OH	1:B:248:ILE:HG23	2.17	0.43
1:A:190:MET:HG2	1:A:209:VAL:HG21	2.01	0.43
1:B:189:LEU:O	1:B:193:LEU:HD13	2.19	0.43
1:B:192:ILE:HD13	1:B:253:GLU:HB3	2.01	0.43
1:B:299[A]:MET:HE1	1:B:329:ILE:HG21	2.01	0.43
1:A:335:ARG:HA	1:A:338:SER:OG	2.19	0.43
1:B:189:LEU:HD12	1:B:192:ILE:CD1	2.44	0.43
1:B:186:THR:HG22	1:B:190:MET:HE3	2.01	0.42
1:A:200:PHE:HZ	1:A:248:ILE:HD13	1.84	0.42
1:B:275:HIS:CE1	1:B:276:GLU:HG3	2.53	0.42
1:B:186:THR:CG2	1:B:209:VAL:HG23	2.49	0.42
1:B:201:VAL:HG12	1:B:201:VAL:O	2.19	0.42
1:B:104:LEU:HD23	1:B:105:LEU:N	2.35	0.42
1:B:354[B]:GLN:NE2	6:B:2058:HOH:O	2.52	0.42
1:A:99[B]:GLU:CG	1:A:128:ASN:HB3	2.49	0.42
1:B:218:TYR:O	1:B:255:PHE:HA	2.19	0.42
1:A:17:VAL:O	1:A:30:VAL:HA	2.20	0.42
1:B:76:ILE:HG21	1:B:79:TRP:CZ3	2.55	0.41
1:B:159:VAL:HG22	1:B:160:THR:N	2.35	0.41
1:B:105:LEU:HD11	1:B:123:MET:CG	2.50	0.41
1:A:175:ILE:O	1:A:176[A]:MET:CE	2.68	0.41
4:A:1377:RH9:H67	4:A:1377:RH9:H781	1.69	0.40
1:B:76:ILE:HD12	1:B:119[B]:MET:CE	2.51	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	358/377 (95%)	348 (97%)	9 (2%)	1 (0%)	46	55
1	B	329/377 (87%)	316 (96%)	11 (3%)	2 (1%)	30	34
All	All	687/754 (91%)	664 (97%)	20 (3%)	3 (0%)	39	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	THR
1	B	201	VAL
1	B	243	PRO

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	308/320 (96%)	303 (98%)	5 (2%)	70	83
1	B	284/320 (89%)	282 (99%)	2 (1%)	88	95
All	All	592/640 (92%)	585 (99%)	7 (1%)	78	89

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ASN
1	A	116	ARG
1	A	189	LEU
1	A	202	THR
1	A	205	GLU
1	B	200	PHE
1	B	205	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	275	HIS
1	A	297	ASN
1	B	225	ASN
1	B	275	HIS
1	B	297	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 10 ligands modelled in this entry, 4 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	A	1375	3	24,33,33	1.11	2 (8%)	31,52,52	1.51	6 (19%)
4	RH9	A	1377	-	92,106,106	1.83	12 (13%)	84,142,142	1.44	10 (11%)
5	HEZ	A	1378	-	7,7,7	0.22	0	6,6,6	0.41	0
5	HEZ	A	1379	-	7,7,7	0.43	0	6,6,6	0.48	0
5	HEZ	A	1380	-	7,7,7	0.42	0	6,6,6	0.26	0
2	ATP	B	1377	3	24,33,33	1.12	2 (8%)	31,52,52	1.83	7 (22%)

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	1375	3	-	0/18/38/38	0/3/3/3
4	RH9	A	1377	-	-	0/140/154/154	0/0/3/3
5	HEZ	A	1378	-	-	0/5/5/5	0/0/0/0
5	HEZ	A	1379	-	-	0/5/5/5	0/0/0/0
5	HEZ	A	1380	-	-	0/5/5/5	0/0/0/0
2	ATP	B	1377	3	-	0/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1377	RH9	C69-N68	-8.53	1.28	1.38
4	A	1377	RH9	C30-N29	-7.81	1.29	1.38
4	A	1377	RH9	C68-N68	-4.45	1.28	1.40
4	A	1377	RH9	C29-N29	-4.42	1.29	1.40
4	A	1377	RH9	C51-C50	-2.48	1.50	1.51
4	A	1377	RH9	O18-C18	-2.09	1.42	1.46
4	A	1377	RH9	C21-C20	2.01	1.55	1.53
4	A	1377	RH9	C58-C59	2.04	1.56	1.52
2	A	1375	ATP	C2-N3	2.08	1.35	1.32
2	B	1377	ATP	C5-C4	2.88	1.47	1.40
2	B	1377	ATP	C2-N3	2.98	1.37	1.32
2	A	1375	ATP	C5-C4	3.13	1.47	1.40
4	A	1377	RH9	C15-C14	3.17	1.51	1.49
4	A	1377	RH9	O58-C1	3.86	1.45	1.34
4	A	1377	RH9	O18-C40	4.22	1.46	1.34
4	A	1377	RH9	C54-C53	6.46	1.53	1.49

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1377	ATP	N3-C2-N1	-5.51	124.67	128.89
2	B	1377	ATP	PA-O3A-PB	-4.22	120.87	132.73
2	A	1375	ATP	N3-C2-N1	-4.18	125.69	128.89
4	A	1377	RH9	C49-C48-C47	-4.10	119.64	125.34
4	A	1377	RH9	C10-C9-C8	-3.72	120.17	125.34
4	A	1377	RH9	C58-C59-C60	-3.14	110.11	114.37
2	B	1377	ATP	C2'-C1'-N9	-2.99	109.72	114.29
4	A	1377	RH9	C36-C21-C20	-2.54	108.48	111.94
2	A	1375	ATP	C2'-C1'-N9	-2.39	110.64	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1375	ATP	C1'-N9-C4	-2.35	123.40	126.94
2	A	1375	ATP	C4'-O4'-C1'	-2.27	107.22	109.72
4	A	1377	RH9	C4-C3-C2	-2.22	108.69	112.94
2	A	1375	ATP	PA-O3A-PB	-2.14	126.72	132.73
2	B	1377	ATP	C4-C5-N7	-2.08	107.57	109.48
4	A	1377	RH9	O40-C40-C41	-2.08	119.92	124.69
2	A	1375	ATP	O2G-PG-O1G	2.02	117.07	110.58
2	B	1377	ATP	O2B-PB-O3A	2.12	114.73	105.09
2	B	1377	ATP	O4'-C1'-N9	2.14	112.58	108.10
4	A	1377	RH9	O58-C1-C2	2.41	116.21	111.54
4	A	1377	RH9	O58-C57-C58	2.74	114.44	107.61
4	A	1377	RH9	C34-C17-C33	3.36	114.28	109.09
2	B	1377	ATP	O3G-PG-O2G	3.45	120.50	107.38
4	A	1377	RH9	O18-C40-C41	4.35	119.96	111.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1377	RH9	2	0
5	A	1378	HEZ	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	358/377 (94%)	1.19	82 (22%) 1 1	37, 54, 69, 89	1 (0%)
1	B	330/377 (87%)	1.81	116 (35%) 0 0	40, 55, 65, 75	0
All	All	688/754 (91%)	1.48	198 (28%) 1 1	37, 55, 66, 89	1 (0%)

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	204	ALA	7.1
1	B	84	LYS	6.7
1	B	91	TYR	6.5
1	B	203	THR	6.4
1	B	363	ASP	6.2
1	A	203	THR	6.0
1	A	64	ILE	5.9
1	B	77	THR	5.9
1	B	158	GLY	5.9
1	A	10	CYS	5.5
1	B	125	GLU	5.4
1	B	80	ASP	5.4
1	B	81	ASP	5.4
1	B	270	GLU	5.4
1	B	199	SER	5.4
1	B	236	LEU	5.4
1	A	365	ALA	5.4
1	B	205	GLU	5.4
1	B	32	PRO	5.3
1	B	245	GLY	5.2
1	A	366	GLY	5.2
1	B	246	GLN	5.0
1	B	202	THR	5.0
1	B	247	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	79	TRP	4.9
1	B	267	ILE	4.9
1	B	225	ASN	4.9
1	B	366	GLY	4.9
1	B	239	SER	4.9
1	B	240	TYR	4.8
1	B	193	LEU	4.8
1	B	251	GLY	4.7
1	B	360	GLN	4.7
1	B	268	GLY	4.5
1	B	78	ASN	4.4
1	B	248	ILE	4.4
1	B	369	ILE	4.3
1	B	231	ALA	4.3
1	B	112	PRO	4.2
1	B	97	ALA	4.2
1	B	194	THR	4.2
1	B	238	LYS	4.1
1	B	252	ASN	4.0
1	A	372	ARG	4.0
1	A	152	VAL	3.9
1	A	151	ILE	3.9
1	A	282	ILE	3.9
1	B	370	VAL	3.9
1	A	258	PRO	3.9
1	B	72	GLU	3.9
1	B	195	GLU	3.9
1	B	323	SER	3.9
1	A	257	CYS	3.9
1	B	324	THR	3.8
1	A	104	LEU	3.8
1	B	201	VAL	3.8
1	B	126	THR	3.7
1	B	95	ARG	3.7
1	B	200	PHE	3.7
1	B	197	GLY	3.7
1	A	199	SER	3.6
1	B	73	HIS	3.6
1	B	241	GLU	3.6
1	A	374	CYS	3.6
1	A	105	LEU	3.5
1	B	265	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	101	HIS	3.5
1	B	249	THR	3.4
1	B	191	LYS	3.4
1	B	222	ASP	3.4
1	B	14	SER	3.4
1	A	243	PRO	3.4
1	A	278	THR	3.4
1	A	255	PHE	3.4
1	A	106	THR	3.3
1	B	190	MET	3.3
1	B	100	GLU	3.3
1	B	188	TYR	3.2
1	B	83	GLU	3.2
1	A	8	LEU	3.2
1	A	270	GLU	3.2
1	A	339	VAL	3.2
1	A	65	LEU	3.1
1	A	5	THR	3.1
1	B	186	THR	3.1
1	A	38	PRO	3.1
1	A	201	VAL	3.1
1	B	198	TYR	3.1
1	B	218	TYR	3.1
1	B	326	LYS	3.1
1	B	212	ILE	3.1
1	B	82	MET	3.0
1	A	9	VAL	3.0
1	B	208	ILE	3.0
1	B	86	TRP	3.0
1	B	178	LEU	3.0
1	B	269	MET	3.0
1	B	117	GLU	3.0
1	B	319	ALA	3.0
1	A	132	MET	2.9
1	A	261	LEU	2.9
1	B	10	CYS	2.9
1	A	340	TRP	2.9
1	A	163	VAL	2.9
1	B	206	ARG	2.9
1	B	257	CYS	2.9
1	B	92	ASN	2.9
1	A	51	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	134	VAL	2.8
1	A	360	GLN	2.8
1	B	151	ILE	2.8
1	B	114	ALA	2.8
1	B	189	LEU	2.8
1	B	192	ILE	2.8
1	B	279	TYR	2.8
1	B	209	VAL	2.8
1	A	103	THR	2.8
1	B	221	LEU	2.8
1	B	287	ILE	2.8
1	A	368	SER	2.7
1	A	343	GLY	2.7
1	B	30	VAL	2.7
1	B	128	ASN	2.7
1	A	298	VAL	2.7
1	B	75	ILE	2.7
1	B	242	LEU	2.7
1	B	367	PRO	2.7
1	A	141	SER	2.7
1	B	163	VAL	2.7
1	A	153	LEU	2.6
1	A	293	LEU	2.6
1	A	19	ALA	2.6
1	B	232	SER	2.6
1	A	299	MET	2.6
1	A	202	THR	2.6
1	A	155	SER	2.6
1	B	15	GLY	2.6
1	B	244	ASP	2.6
1	A	129	VAL	2.6
1	A	369	ILE	2.5
1	A	217	CYS	2.5
1	A	304	THR	2.5
1	B	368	SER	2.5
1	A	371	HIS	2.5
1	B	229	THR	2.5
1	A	185	LEU	2.5
1	A	164	PRO	2.5
1	A	370	VAL	2.5
1	B	228	ALA	2.5
1	A	17	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	311	ASP	2.5
1	B	220	ALA	2.4
1	B	104	LEU	2.4
1	A	53	TYR	2.4
1	B	365	ALA	2.4
1	A	142	LEU	2.4
1	A	160	THR	2.4
1	A	204	ALA	2.4
1	A	347	ALA	2.4
1	A	367	PRO	2.4
1	B	372	ARG	2.4
1	A	219	VAL	2.4
1	A	344	SER	2.4
1	A	156	GLY	2.3
1	B	87	HIS	2.3
1	A	262	PHE	2.3
1	B	207	GLU	2.3
1	B	362	TYR	2.3
1	B	226	GLU	2.3
1	A	297	ASN	2.3
1	B	216	LEU	2.3
1	B	224	GLU	2.3
1	B	181	ALA	2.3
1	B	183	ARG	2.2
1	B	299[A]	MET	2.2
1	A	274	ILE	2.2
1	B	350	SER	2.2
1	A	138	ALA	2.2
1	B	196	ARG	2.2
1	A	338	SER	2.2
1	A	287	ILE	2.2
1	B	6	THR	2.2
1	A	144	ALA	2.2
1	A	154	ASP	2.1
1	A	232	SER	2.1
1	B	266	PHE	2.1
1	A	119	MET	2.1
1	A	189	LEU	2.1
1	A	62	ARG	2.1
1	A	342	GLY	2.1
1	B	210	ARG	2.1
1	B	271	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	2.1
1	A	162	ASN	2.1
1	A	281	SER	2.1
1	A	300	SER	2.0
1	A	301	GLY	2.0
1	A	200	PHE	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, 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(Å ²)	Q<0.9
5	HEZ	A	1380	8/8	0.74	0.51	9.98	76,77,82,84	0
5	HEZ	A	1378	8/8	0.86	0.20	1.06	31,36,46,47	1
5	HEZ	A	1379	8/8	0.80	0.15	-0.30	70,71,73,74	0
2	ATP	B	1377	31/31	0.94	0.13	-1.24	53,61,68,69	0
4	RH9	A	1377	104/104	0.94	0.12	-1.25	33,42,48,50	0
3	CA	B	1376	1/1	0.81	0.14	-1.27	61,61,61,61	0
2	ATP	A	1375	31/31	0.97	0.14	-1.65	33,39,41,42	0
3	CA	A	1376	1/1	0.99	0.10	-4.84	35,35,35,35	0
3	CA	B	1378	1/1	0.97	0.05	-5.63	54,54,54,54	0
3	CA	B	1379	1/1	0.36	0.14	-	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.