



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3A37  
Title : Structural insight into the membrane insertion of tail-anchored proteins by Get3  
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Deposited on : 2009-06-10  
Resolution : 3.00 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

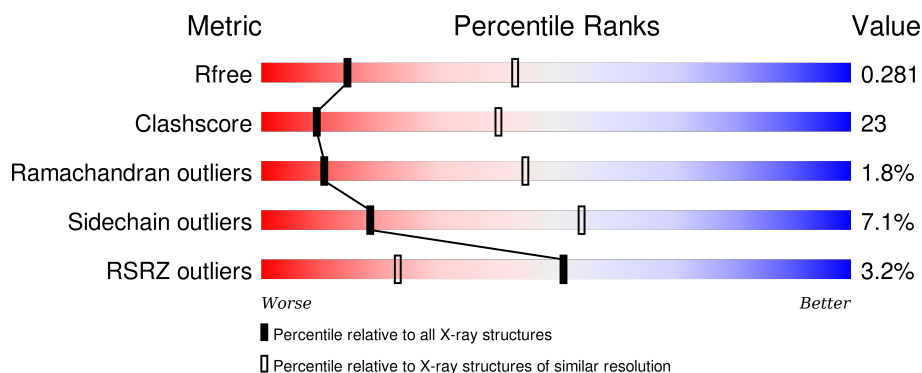
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	362	<div> <div>2%</div> <div>47%</div> <div>35%</div> <div>•</div> <div>14%</div> </div>
1	B	362	<div> <div>3%</div> <div>53%</div> <div>32%</div> <div>•</div> <div>12%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4925 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2398	1514	401	467	16			
1	B	319	Total	C	N	O	S	0	0	0
			2472	1560	414	481	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ASP	GLY	CONFLICT	UNP Q12154
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	155	ASP	GLY	CONFLICT	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.23Å 222.55Å 49.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.00 49.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.29-3.00) 97.3 (49.29-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.253 , 0.282 0.253 , 0.281	Depositor DCC
$R_{free}$ test set	1233 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 25702 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4925	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% 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: ZN, ADP

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	0.43	0/2438	0.68	2/3297 (0.1%)
1	B	0.45	0/2510	0.66	0/3389
All	All	0.44	0/4948	0.67	2/6686 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	275	LEU	CA-CB-CG	5.47	127.88	115.30
1	A	52	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	TYR	Sidechain

### 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	2398	0	2330	134	0
1	B	2472	0	2442	90	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
3	A	1	0	0	0	0
All	All	4925	0	4796	221	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 23.

All (221) 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:242:CYS:HB3	1:A:252:THR:HG21	1.37	1.04
1:B:20:TRP:HB2	1:B:236:THR:HB	1.50	0.94
1:B:52:LEU:HD21	1:B:86:MET:HG2	1.50	0.93
1:A:8:ASN:HA	1:A:312:VAL:HG22	1.55	0.88
1:B:243:ILE:HD12	1:B:244:SER:H	1.36	0.88
1:A:287:ARG:HG2	1:A:287:ARG:HH11	1.36	0.87
1:B:13:ILE:HD13	1:B:41:GLN:HG2	1.58	0.85
1:A:291:ARG:NH1	1:B:291:ARG:HD3	1.91	0.85
1:B:40:ILE:HG21	1:B:328:THR:HG22	1.57	0.84
1:B:324:LEU:O	1:B:328:THR:HG23	1.78	0.84
1:B:230:PHE:HA	1:B:236:THR:HG21	1.62	0.80
1:A:129:LEU:HD12	1:A:129:LEU:H	1.46	0.80
1:B:133:ILE:HB	1:B:136:ILE:HD12	1.65	0.79
1:B:262:TYR:O	1:B:263:ASP:HB2	1.81	0.79
1:A:254:ARG:HB3	1:A:254:ARG:HH11	1.48	0.78
1:A:52:LEU:HD12	1:A:163:VAL:HG22	1.64	0.78
1:B:121:LEU:HA	1:B:215:LYS:HD2	1.66	0.78
1:B:130:THR:HG23	1:B:137:ASP:HB2	1.66	0.78
1:A:8:ASN:HD22	1:A:10:HIS:H	1.29	0.78
1:A:227:ARG:O	1:A:231:THR:HB	1.85	0.76
1:A:80:MET:HG2	1:A:324:LEU:HD11	1.68	0.75
1:B:227:ARG:O	1:B:231:THR:HB	1.87	0.75
1:B:253:GLU:HG2	1:B:306:TYR:OH	1.87	0.74
1:A:249:LEU:HD21	1:A:302:ILE:HD11	1.68	0.73
1:B:287:ARG:HH11	1:B:287:ARG:HG3	1.53	0.72
1:A:292:TRP:CE2	1:A:296:LYS:HD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:HA	1:A:294:MET:HE3	1.73	0.71
1:A:180:PRO:HD3	1:A:223:VAL:HG11	1.73	0.71
1:A:291:ARG:HD3	1:B:291:ARG:NH1	2.06	0.70
1:A:275:LEU:HD23	1:A:295:GLN:OE1	1.92	0.70
1:A:36:CYS:O	1:A:40:ILE:HG13	1.94	0.68
1:A:52:LEU:HB2	1:A:160:PHE:CD2	2.29	0.68
1:A:209:ASN:O	1:A:212:ILE:HB	1.94	0.66
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.08	0.66
1:A:255:LEU:HD22	1:A:259:LEU:CD1	2.26	0.66
1:B:324:LEU:HD12	1:B:328:THR:HG23	1.77	0.66
1:A:138:GLU:OE2	1:A:175:ARG:NH1	2.30	0.64
1:A:232:ASP:OD2	1:A:235:LEU:HG	1.97	0.64
1:A:130:THR:HG23	1:A:137:ASP:HB2	1.80	0.63
1:A:270:ILE:HG13	1:A:270:ILE:O	1.96	0.63
1:A:20:TRP:HB2	1:A:236:THR:CG2	2.28	0.63
1:B:292:TRP:NE1	1:B:296:LYS:HD2	2.13	0.63
1:A:70:PHE:CD2	1:A:85:CYS:HB2	2.34	0.62
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.81	0.62
1:A:257:GLN:HA	1:A:257:GLN:OE1	1.99	0.62
1:A:221:ALA:O	1:A:225:THR:HG23	2.00	0.62
1:A:175:ARG:HH11	1:A:175:ARG:HB3	1.63	0.61
1:A:60:HIS:HA	1:A:87:GLU:OE1	2.02	0.60
1:A:262:TYR:O	1:A:263:ASP:HB2	2.01	0.60
1:A:6:GLU:O	1:A:310:HIS:HD2	1.83	0.60
1:A:74:ALA:HB2	1:A:86:MET:CE	2.32	0.59
1:A:70:PHE:CE2	1:A:85:CYS:HB2	2.37	0.59
1:B:100:MET:CE	1:B:104:ARG:HE	2.14	0.59
1:B:243:ILE:HD12	1:B:244:SER:N	2.13	0.59
1:A:5:VAL:HG12	1:A:310:HIS:CD2	2.38	0.59
1:B:230:PHE:HA	1:B:236:THR:CG2	2.30	0.58
1:A:129:LEU:HD12	1:A:129:LEU:N	2.17	0.58
1:A:254:ARG:CB	1:A:254:ARG:HH11	2.16	0.58
1:A:8:ASN:ND2	1:A:10:HIS:H	1.99	0.58
1:B:221:ALA:O	1:B:225:THR:HG23	2.04	0.58
1:A:8:ASN:CA	1:A:312:VAL:HG22	2.32	0.58
1:B:13:ILE:HD13	1:B:41:GLN:CG	2.29	0.58
1:B:324:LEU:HD12	1:B:328:THR:CG2	2.33	0.58
1:A:329:LYS:O	1:A:332:GLN:HG2	2.04	0.58
1:A:345:LYS:HA	1:A:345:LYS:HE2	1.86	0.57
1:A:242:CYS:CB	1:A:252:THR:HG21	2.24	0.57
1:A:8:ASN:HA	1:A:312:VAL:CG2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:THR:HG23	1:A:18:HIS:ND1	2.20	0.56
1:B:282:GLU:C	1:B:284:ASN:H	2.09	0.56
1:A:133:ILE:HB	1:A:136:ILE:CD1	2.36	0.56
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.88	0.56
1:A:282:GLU:C	1:A:284:ASN:H	2.09	0.56
1:A:80:MET:HE3	1:A:83:LEU:CB	2.36	0.55
1:A:174:LEU:H	1:A:174:LEU:HD23	1.71	0.55
1:B:180:PRO:HD3	1:B:223:VAL:HG11	1.89	0.55
1:A:245:GLU:HG2	1:A:294:MET:CE	2.36	0.55
1:B:278:GLU:O	1:B:280:ASP:N	2.40	0.55
1:A:347:ILE:HD12	1:A:347:ILE:C	2.28	0.55
1:B:54:ILE:HD11	1:B:149:ILE:HG12	1.88	0.55
1:B:174:LEU:CD2	1:B:174:LEU:H	2.21	0.54
1:B:285:CYS:O	1:B:289:GLN:HG2	2.06	0.54
1:A:177:LEU:HD12	1:A:262:TYR:HB3	1.88	0.54
1:B:185:LYS:O	1:B:188:GLU:HG2	2.08	0.54
1:B:243:ILE:HD13	1:B:272:ASN:O	2.08	0.54
1:A:272:ASN:ND2	1:A:273:GLN:HG3	2.22	0.54
1:B:320:GLU:OE2	1:B:322:ARG:HD3	2.08	0.54
1:A:210:VAL:HG12	1:A:210:VAL:O	2.08	0.53
1:B:183:LEU:HD12	1:B:220:LYS:HB2	1.90	0.53
1:B:16:THR:HG22	1:B:46:GLN:NE2	2.24	0.53
1:A:245:GLU:HG2	1:A:294:MET:HE1	1.90	0.52
1:A:138:GLU:OE1	1:A:138:GLU:N	2.40	0.52
1:A:88:ILE:HG22	1:A:89:ASP:N	2.25	0.52
1:A:256:ILE:O	1:A:260:ILE:HG13	2.10	0.52
1:A:31:LYS:HE2	1:A:167:THR:O	2.10	0.52
1:B:345:LYS:O	1:B:349:GLU:HG3	2.10	0.51
1:A:175:ARG:HH11	1:A:175:ARG:CB	2.21	0.51
1:A:238:PHE:CD2	1:A:259:LEU:HD11	2.46	0.51
1:A:20:TRP:HB2	1:A:236:THR:HG22	1.92	0.51
1:A:13:ILE:HD13	1:A:41:GLN:HG2	1.93	0.51
1:B:6:GLU:O	1:B:310:HIS:HD2	1.93	0.51
1:B:274:LEU:HD21	1:B:299:LEU:HD21	1.92	0.51
1:A:179:LEU:HD23	1:A:223:VAL:HG21	1.93	0.50
1:A:249:LEU:CD2	1:A:302:ILE:HD11	2.37	0.50
1:B:126:LEU:HD22	1:B:215:LYS:HB3	1.93	0.50
1:A:20:TRP:CD1	1:A:236:THR:HG22	2.45	0.50
1:A:54:ILE:HD11	1:A:88:ILE:HD12	1.93	0.50
1:A:129:LEU:CD1	1:A:129:LEU:H	2.20	0.50
1:A:345:LYS:O	1:A:349:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:HD12	1:A:42:MET:CE	2.42	0.50
1:A:9:LEU:HD12	1:A:334:LEU:HD13	1.93	0.50
1:B:172:HIS:HB2	1:B:175:ARG:HH21	1.77	0.50
1:A:292:TRP:NE1	1:A:296:LYS:HD2	2.28	0.49
1:B:94:LEU:HD12	1:B:141:SER:HA	1.94	0.49
1:B:34:SER:O	1:B:38:ILE:HG13	2.13	0.49
1:A:80:MET:HE3	1:A:83:LEU:HB2	1.95	0.49
1:A:64:ASP:O	1:A:322:ARG:HD3	2.13	0.49
1:A:255:LEU:HD22	1:A:259:LEU:HD11	1.95	0.48
1:A:175:ARG:NH1	1:A:175:ARG:CB	2.76	0.48
1:B:174:LEU:CD2	1:B:174:LEU:N	2.77	0.48
1:A:229:GLN:OE1	1:A:235:LEU:HD13	2.13	0.48
1:B:164:ILE:HD12	1:B:164:ILE:N	2.28	0.48
1:B:324:LEU:O	1:B:324:LEU:HD12	2.13	0.48
1:A:20:TRP:HD1	1:A:236:THR:HG22	1.77	0.48
1:B:222:ASN:O	1:B:226:ILE:HG13	2.13	0.48
1:B:3:LEU:HD23	1:B:3:LEU:N	2.29	0.48
1:B:13:ILE:HG21	1:B:41:GLN:HG3	1.94	0.48
1:B:51:PHE:CD2	1:B:162:THR:HB	2.49	0.48
1:A:287:ARG:CG	1:A:287:ARG:NH1	2.76	0.48
1:A:13:ILE:HA	1:A:42:MET:HG3	1.96	0.48
1:B:255:LEU:CD2	1:B:259:LEU:HG	2.44	0.47
1:A:174:LEU:CD2	1:A:174:LEU:H	2.27	0.47
1:B:19:LYS:NZ	1:B:229:GLN:NE2	2.61	0.47
1:B:294:MET:O	1:B:297:LYS:HB3	2.15	0.47
1:B:20:TRP:O	1:B:236:THR:HA	2.14	0.47
1:A:50:GLN:NE2	1:A:82:ASN:HA	2.30	0.47
1:B:133:ILE:HB	1:B:136:ILE:CD1	2.41	0.47
1:B:10:HIS:O	1:B:14:THR:HB	2.14	0.47
1:A:22:PHE:CE1	1:A:165:PHE:CD1	3.03	0.47
1:B:174:LEU:H	1:B:174:LEU:HD23	1.79	0.47
1:A:285:CYS:O	1:A:289:GLN:HG2	2.15	0.47
1:B:232:ASP:HB3	1:B:235:LEU:HB2	1.97	0.47
1:A:7:PRO:HG2	1:A:337:GLU:OE1	2.15	0.47
1:A:34:SER:OG	1:A:270:ILE:HD11	2.15	0.46
1:A:19:LYS:HD3	1:A:235:LEU:HD22	1.97	0.46
1:A:248:SER:O	1:A:252:THR:HG23	2.16	0.46
1:B:278:GLU:C	1:B:280:ASP:H	2.18	0.46
1:A:238:PHE:CE2	1:A:259:LEU:HD11	2.50	0.46
1:B:287:ARG:HG3	1:B:287:ARG:NH1	2.26	0.46
1:B:46:GLN:HE21	1:B:49:LYS:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:TRP:O	1:A:236:THR:HA	2.16	0.46
1:A:256:ILE:HD13	1:A:309:PHE:HE1	1.81	0.46
1:A:176:PHE:C	1:A:176:PHE:CD2	2.89	0.45
1:A:27:GLY:HA2	1:B:246:PHE:CD2	2.50	0.45
1:A:222:ASN:HD22	1:A:222:ASN:HA	1.56	0.45
1:B:100:MET:HE3	1:B:104:ARG:HE	1.81	0.45
1:A:181:ASN:OD1	1:A:185:LYS:HE3	2.16	0.45
1:A:6:GLU:O	1:A:310:HIS:CD2	2.68	0.45
1:A:332:GLN:HG3	1:A:333:PHE:CD2	2.52	0.45
1:A:146:MET:O	1:A:150:LYS:HG3	2.17	0.45
1:B:68:GLU:OE1	1:B:78:THR:HB	2.16	0.45
1:B:124:GLY:O	1:B:125:ALA:HB2	2.17	0.45
1:A:230:PHE:CD1	1:A:230:PHE:N	2.85	0.45
1:A:52:LEU:HD12	1:A:163:VAL:CG2	2.41	0.44
1:A:246:PHE:C	1:A:246:PHE:CD2	2.89	0.44
1:A:128:ASP:C	1:A:130:THR:H	2.18	0.44
1:B:90:PRO:O	1:B:94:LEU:HB2	2.18	0.44
1:B:51:PHE:CE2	1:B:162:THR:HB	2.52	0.44
1:B:150:LYS:HB3	1:B:150:LYS:NZ	2.32	0.44
1:B:287:ARG:O	1:B:290:ALA:HB3	2.17	0.44
1:B:72:LYS:HA	1:B:88:ILE:HG22	2.00	0.44
1:B:31:LYS:HD2	1:B:166:ASP:OD1	2.18	0.44
1:B:317:CYS:HB2	2:B:401:ADP:C2	2.52	0.44
1:A:232:ASP:HB3	1:A:235:LEU:HB2	2.00	0.43
1:B:282:GLU:O	1:B:284:ASN:N	2.51	0.43
1:B:70:PHE:CD2	1:B:85:CYS:HB2	2.53	0.43
1:A:80:MET:HE3	1:A:83:LEU:HB3	2.01	0.43
1:B:145:VAL:O	1:B:149:ILE:HG13	2.19	0.43
1:A:347:ILE:HD11	1:A:348:TYR:CZ	2.54	0.43
1:A:20:TRP:O	1:A:236:THR:HB	2.19	0.43
1:A:347:ILE:HD12	1:A:347:ILE:O	2.19	0.42
1:A:65:ALA:O	1:A:322:ARG:HG3	2.19	0.42
1:A:280:ASP:C	1:A:282:GLU:N	2.72	0.42
1:B:149:ILE:O	1:B:153:GLU:HG3	2.19	0.42
1:B:20:TRP:HE1	1:B:229:GLN:HE21	1.67	0.42
1:A:133:ILE:HB	1:A:136:ILE:HD12	2.01	0.42
1:B:275:LEU:O	1:B:277:ALA:N	2.52	0.42
1:A:43:ALA:HA	1:A:51:PHE:CD1	2.55	0.42
1:B:231:THR:O	1:B:231:THR:CG2	2.68	0.42
1:A:256:ILE:HD12	1:A:306:TYR:CE2	2.54	0.42
1:B:249:LEU:O	1:B:249:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD13	1:A:41:GLN:CG	2.49	0.42
1:B:43:ALA:HA	1:B:51:PHE:CE1	2.54	0.42
1:B:19:LYS:NZ	1:B:229:GLN:HE22	2.17	0.42
1:A:314:MET:SD	1:A:334:LEU:HD23	2.60	0.42
1:B:19:LYS:HZ3	1:B:229:GLN:HE22	1.68	0.41
1:A:75:ARG:HE	1:A:75:ARG:HB3	1.66	0.41
1:B:278:GLU:HG3	1:B:292:TRP:CD1	2.55	0.41
1:A:15:SER:OG	1:A:17:THR:HG22	2.19	0.41
1:B:94:LEU:O	1:B:94:LEU:HD23	2.20	0.41
1:B:264:MET:HG3	1:B:265:ASP:N	2.34	0.41
1:A:238:PHE:CD2	1:A:259:LEU:CD1	3.02	0.41
1:B:238:PHE:CG	1:B:259:LEU:HD11	2.56	0.41
1:A:259:LEU:HD22	1:A:264:MET:HG2	2.01	0.41
1:B:324:LEU:CD1	1:B:328:THR:CG2	2.98	0.41
1:A:251:GLU:OE2	1:A:254:ARG:NH1	2.53	0.41
1:A:156:GLU:O	1:A:158:GLU:N	2.54	0.41
1:A:174:LEU:CD2	1:A:174:LEU:N	2.83	0.41
1:A:344:GLY:O	1:A:348:TYR:CD2	2.74	0.41
1:A:172:HIS:O	1:A:174:LEU:N	2.54	0.41
1:B:212:ILE:HG22	1:B:213:SER:N	2.36	0.41
1:A:128:ASP:C	1:A:130:THR:N	2.74	0.40
1:A:74:ALA:HB2	1:A:86:MET:HE3	2.03	0.40
1:A:164:ILE:HD12	1:A:164:ILE:N	2.36	0.40
1:A:275:LEU:O	1:A:277:ALA:N	2.54	0.40
1:A:255:LEU:HD22	1:A:259:LEU:HD12	2.03	0.40
1:A:20:TRP:HB2	1:A:236:THR:HB	2.02	0.40
1:B:35:SER:HB3	1:B:53:LEU:HD11	2.03	0.40
1:A:282:GLU:O	1:A:284:ASN:N	2.51	0.40
1:B:13:ILE:HA	1:B:42:MET:HG2	2.03	0.40
1:A:241:VAL:HG22	1:A:270:ILE:HG12	2.03	0.40
1:A:314:MET:HE2	1:A:330:PHE:CZ	2.57	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	309/362 (85%)	278 (90%)	26 (8%)	5 (2%)	12	48
1	B	313/362 (86%)	283 (90%)	24 (8%)	6 (2%)	10	43
All	All	622/724 (86%)	561 (90%)	50 (8%)	11 (2%)	11	45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	THR
1	B	173	THR
1	B	283	HIS
1	A	280	ASP
1	A	285	CYS
1	B	279	ASN
1	B	125	ALA
1	B	157	GLY
1	A	283	HIS
1	B	123	GLY
1	A	157	GLY

### 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	260/318 (82%)	242 (93%)	18 (7%)	19	56
1	B	274/318 (86%)	254 (93%)	20 (7%)	17	52
All	All	534/636 (84%)	496 (93%)	38 (7%)	18	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU

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Mol	Chain	Res	Type
1	A	31	LYS
1	A	45	SER
1	A	129	LEU
1	A	159	THR
1	A	174	LEU
1	A	222	ASN
1	A	231	THR
1	A	253	GLU
1	A	254	ARG
1	A	255	LEU
1	A	270	ILE
1	A	274	LEU
1	A	291	ARG
1	A	313	LYS
1	A	324	LEU
1	A	329	LYS
1	B	12	LEU
1	B	14	THR
1	B	52	LEU
1	B	64	ASP
1	B	84	SER
1	B	121	LEU
1	B	151	ARG
1	B	174	LEU
1	B	179	LEU
1	B	236	THR
1	B	239	VAL
1	B	243	ILE
1	B	274	LEU
1	B	275	LEU
1	B	287	ARG
1	B	291	ARG
1	B	312	VAL
1	B	313	LYS
1	B	315	PRO
1	B	337	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	41	GLN

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Mol	Chain	Res	Type
1	A	50	GLN
1	A	178	GLN
1	A	222	ASN
1	A	273	GLN
1	A	310	HIS
1	B	46	GLN
1	B	50	GLN
1	B	60	HIS
1	B	107	ASN
1	B	178	GLN
1	B	229	GLN
1	B	267	ASN
1	B	310	HIS
1	B	332	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](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	ADP	A	400	-	22,29,29	1.82	4 (18%)	27,45,45	2.90	4 (14%)
2	ADP	B	401	-	22,29,29	1.81	5 (22%)	27,45,45	2.86	2 (7%)

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	ADP	A	400	-	-	0/12/32/32	0/3/3/3
2	ADP	B	401	-	-	0/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	ADP	C5-N7	-3.23	1.28	1.39
2	B	401	ADP	C5-N7	-3.15	1.28	1.39
2	B	401	ADP	PA-O2A	-2.40	1.44	1.54
2	A	400	ADP	C5-C4	2.05	1.45	1.40
2	B	401	ADP	C5'-C4'	2.05	1.58	1.51
2	B	401	ADP	C2-N1	3.53	1.40	1.33
2	A	400	ADP	C2-N1	3.72	1.41	1.33
2	B	401	ADP	C2-N3	4.52	1.40	1.32
2	A	400	ADP	C2-N3	5.00	1.41	1.32

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ADP	N3-C2-N1	-13.80	118.33	128.89
2	A	400	ADP	N3-C2-N1	-13.58	118.50	128.89
2	A	400	ADP	C4-C5-N7	-2.29	107.37	109.48
2	B	401	ADP	C4'-O4'-C1'	2.29	112.24	109.72
2	A	400	ADP	C2'-C3'-C4'	2.54	107.83	102.61
2	A	400	ADP	C4'-O4'-C1'	3.69	113.77	109.72

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
2	B	401	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	313/362 (86%)	0.09	8 (2%) 59 29	58, 91, 139, 155	0
1	B	319/362 (88%)	0.03	12 (3%) 44 18	54, 84, 143, 159	0
All	All	632/724 (87%)	0.06	20 (3%) 51 23	54, 88, 140, 159	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ILE	5.1
1	B	122	GLN	4.4
1	B	119	SER	3.6
1	B	211	ASP	3.4
1	B	121	LEU	3.2
1	A	212	ILE	3.1
1	B	186	LEU	3.1
1	B	190	PHE	3.0
1	A	186	LEU	3.0
1	B	191	GLY	2.7
1	A	279	ASN	2.7
1	A	216	LEU	2.5
1	A	90	PRO	2.4
1	B	126	LEU	2.3
1	A	286	LYS	2.2
1	B	284	ASN	2.1
1	B	179	LEU	2.1
1	A	136	ILE	2.1
1	B	187	LEU	2.1
1	A	187	LEU	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(Å <sup>2</sup> )	Q<0.9
2	ADP	B	401	27/27	0.89	0.25	0.03	93,100,103,104	0
3	ZN	A	363	1/1	0.99	0.12	-1.02	97,97,97,97	0
2	ADP	A	400	27/27	0.95	0.18	-1.27	97,105,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.