



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:29 PM GMT

PDB ID : 4XVU  
Title : Structure of Get3 bound to the transmembrane domain of Nyv1  
Authors : Mateja, A.; Paduch, M.; Chang, H.-Y.; Szydlowska, A.; Kossiakoff, A.A.; Hegde, R.S.; Keenan, R.J.  
Deposited on : 2015-01-28  
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](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

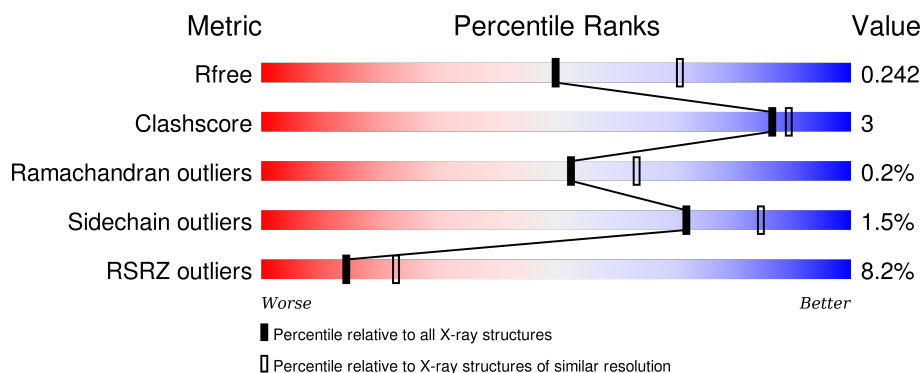
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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  $\geq 3$ , 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	354	<div> <div>5%</div> <div>80%</div> <div>5%</div> <div>15%</div> </div>
1	B	354	<div> <div>4%</div> <div>79%</div> <div>6%</div> <div>14%</div> </div>
1	G	354	<div> <div>5%</div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	H	354	<div> <div>6%</div> <div>80%</div> <div>8%</div> <div>12%</div> </div>
2	C	230	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	230	<div><div></div><div>3%</div><div>94%</div><div></div><div></div></div>
2	I	230	<div><div></div><div>13%</div><div>83%</div><div>7%</div><div>10%</div></div>
2	K	230	<div><div></div><div>18%</div><div>80%</div><div>11%</div><div>6%</div></div>
3	D	217	<div><div></div><div>%</div><div>95%</div><div></div><div></div></div>
3	F	217	<div><div></div><div></div><div>93%</div><div></div><div>6%</div></div>
3	J	217	<div><div></div><div>23%</div><div>91%</div><div></div><div>8%</div></div>
3	L	217	<div><div></div><div>15%</div><div>90%</div><div></div><div>9%</div></div>
4	a	37	<div><div></div><div>68%</div><div></div><div>32%</div></div>
4	g	37	<div><div></div><div>32%</div><div>68%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 46586 atoms, of which 22641 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	301	Total	C	H	N	O	S	0	2	0
			4764	1512	2373	397	464	18			
1	B	304	Total	C	H	N	O	S	0	1	0
			4794	1521	2387	399	469	18			
1	G	307	Total	C	H	N	O	S	0	0	0
			4835	1535	2408	403	473	16			
1	H	311	Total	C	H	N	O	S	0	0	0
			4887	1549	2436	408	477	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	ASN	ASP	engineered mutation	UNP Q12154
B	57	ASN	ASP	engineered mutation	UNP Q12154
G	57	ASN	ASP	engineered mutation	UNP Q12154
H	57	ASN	ASP	engineered mutation	UNP Q12154

- Molecule 2 is a protein called Antibody heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	222	Total	C	H	N	O	S	0	0	0
			3289	1050	1625	282	326	6			
2	E	222	Total	C	H	N	O	S	0	0	0
			3289	1050	1625	282	326	6			
2	I	207	Total	C	H	N	O	S	0	0	0
			3097	996	1529	265	301	6			
2	K	216	Total	C	H	N	O	S	0	0	0
			3213	1029	1587	275	316	6			

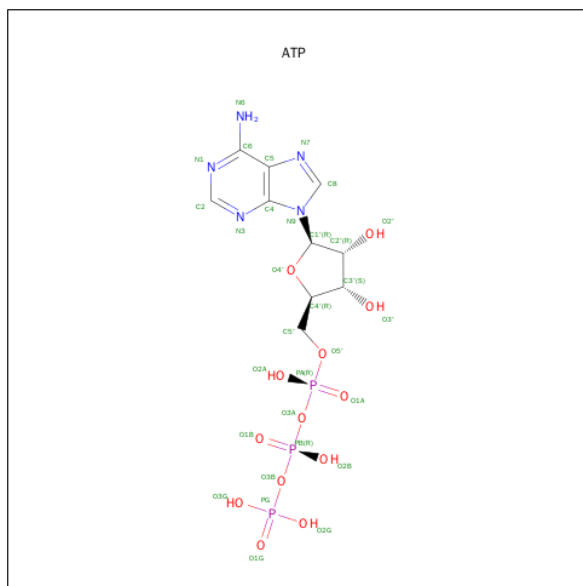
- Molecule 3 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	216	Total	C	H	N	O	S	0	0	0
			3269	1038	1611	276	338	6			
3	F	216	Total	C	H	N	O	S	0	0	0
			3269	1038	1611	276	338	6			
3	J	215	Total	C	H	N	O	S	0	0	0
			3257	1034	1607	275	335	6			
3	L	216	Total	C	H	N	O	S	0	0	0
			3269	1038	1611	276	338	6			

- Molecule 4 is a protein called Nyv1 TMD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	g	12	Total	C	H	N	O	0	0	0
			119	36	59	12	12			
4	a	25	Total	C	H	N	O	0	0	0
			252	75	127	25	25			

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



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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	H	1	Total	C	H	N	O	P	0	0
			43	10	12	5	13	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	G	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Zn	0	0
			1	1		
7	A	1	Total	Zn	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	57	Total	O	0	0
			57	57		
8	B	85	Total	O	0	0
			85	85		
8	C	62	Total	O	0	0
			62	62		
8	D	77	Total	O	0	0
			77	77		
8	E	52	Total	O	0	0
			52	52		
8	F	93	Total	O	0	0
			93	93		
8	G	107	Total	O	0	0
			107	107		
8	H	85	Total	O	0	0
			85	85		

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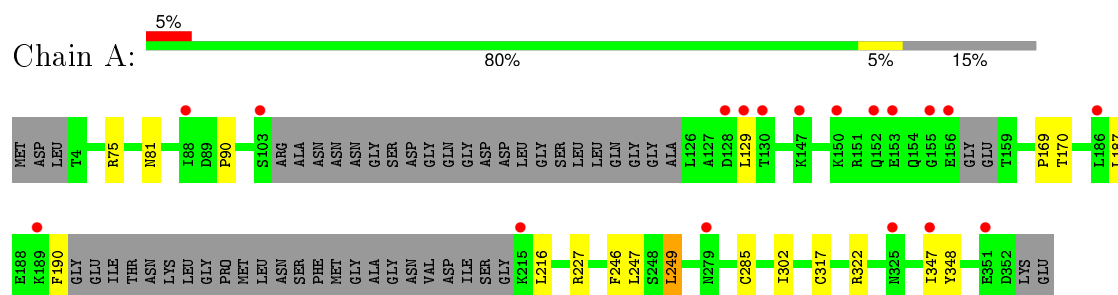
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	I	42	Total 42	O 42	0	0
8	J	45	Total 45	O 45	0	0
8	K	61	Total 61	O 61	0	0
8	L	42	Total 42	O 42	0	0

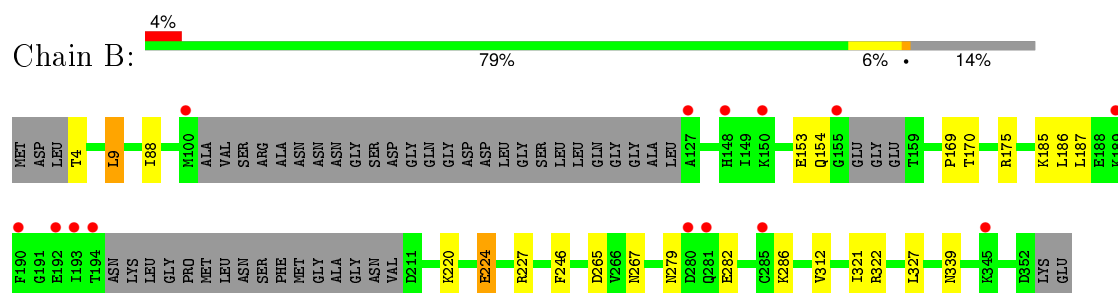
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

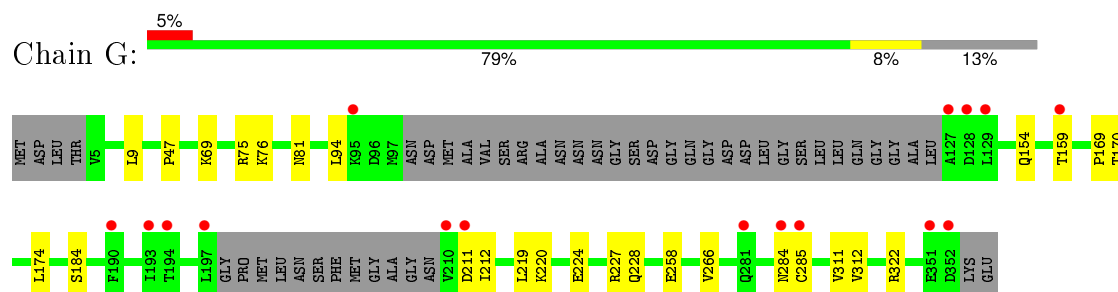
#### • Molecule 1: ATPase GET3



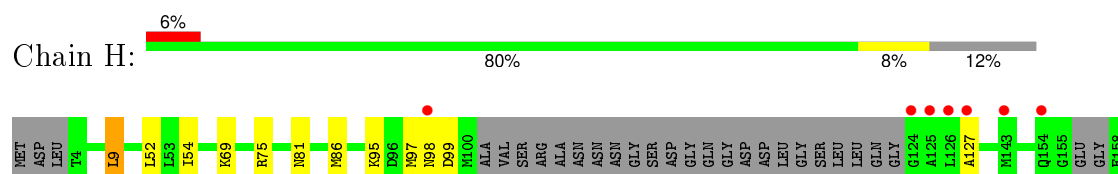
#### • Molecule 1: ATPase GET3



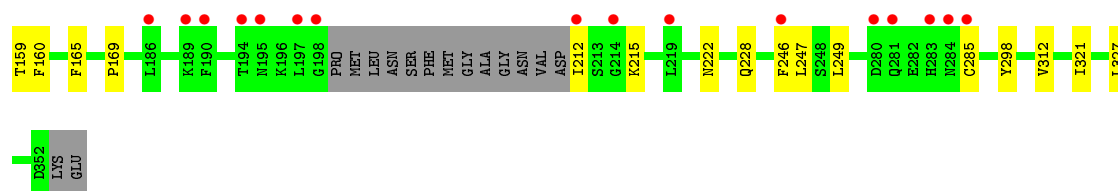
#### • Molecule 1: ATPase GET3



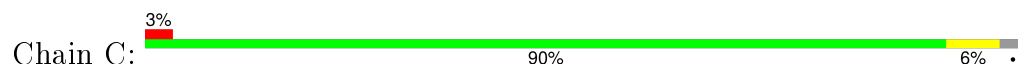
#### • Molecule 1: ATPase GET3







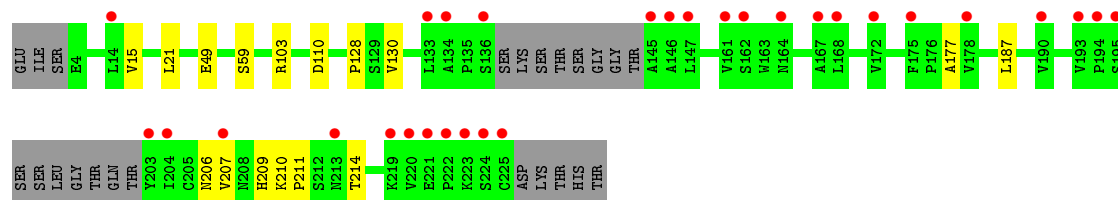
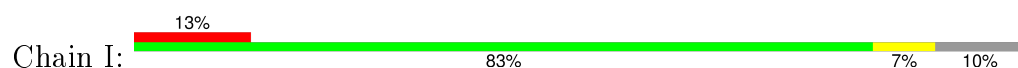
- Molecule 2: Antibody heavy chain



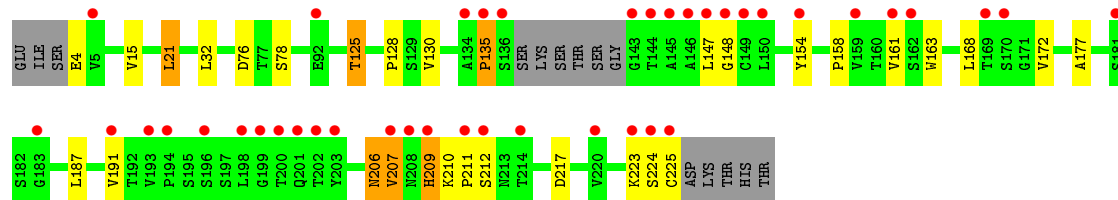
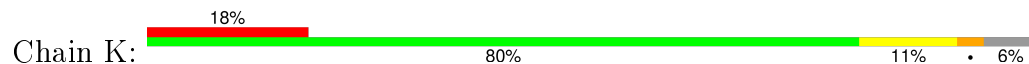
- Molecule 2: Antibody heavy chain



- Molecule 2: Antibody heavy chain



- Molecule 2: Antibody heavy chain



- Molecule 3: Antibody light chain




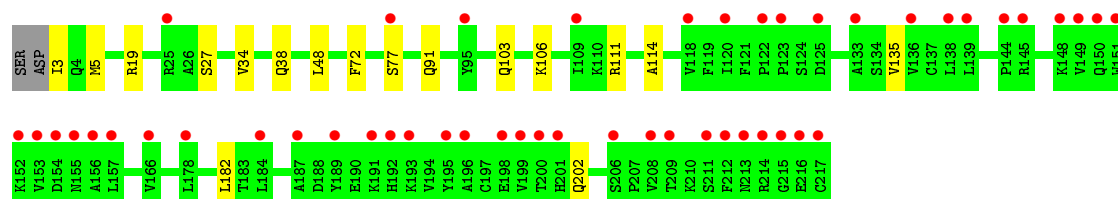
- Molecule 3: Antibody light chain

Chain F:  93% 6%




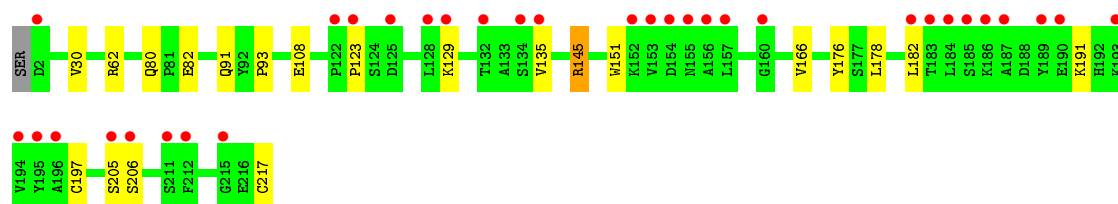
- Molecule 3: Antibody light chain

Chain J:  23% 91% 8%



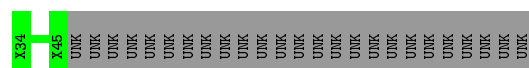
- Molecule 3: Antibody light chain

Chain L:  15% 90% 9%



- Molecule 4: Nyv1 TMD

Chain g:  32% 68%



- Molecule 4: Nyv1 TMD

Chain a:  68% 32%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.44Å 109.23Å 111.35Å 63.05° 77.74° 70.17°	Depositor
Resolution (Å)	69.38 – 2.35 69.38 – 2.35	Depositor EDS
% Data completeness (in resolution range)	94.6 (69.38-2.35) 78.2 (69.38-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.197 , 0.234 0.208 , 0.242	Depositor DCC
$R_{free}$ test set	6209 reflections (5.51%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.2	Xtriage
Anisotropy	0.303	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123345 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	46586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, ZN, 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	0.28	0/2437	0.42	0/3287
1	B	0.27	0/2449	0.44	0/3302
1	G	0.29	0/2467	0.43	0/3327
1	H	0.27	0/2490	0.42	0/3356
2	C	0.30	0/1706	0.52	0/2326
2	E	0.29	0/1706	0.52	0/2326
2	I	0.27	0/1608	0.49	0/2191
2	K	0.31	0/1667	0.58	0/2273
3	D	0.29	0/1694	0.49	0/2299
3	F	0.33	0/1694	0.56	0/2299
3	J	0.27	0/1686	0.49	0/2288
3	L	0.30	0/1694	0.55	1/2299 (0.0%)
All	All	0.29	0/23298	0.49	1/31573 (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
3	F	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	145	ARG	NE-CZ-NH1	7.12	123.86	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	146	GLU	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	2391	2373	2364	12	0
1	B	2407	2387	2387	14	0
1	G	2427	2408	2411	15	1
1	H	2451	2436	2436	18	0
2	C	1664	1625	1625	9	0
2	E	1664	1625	1625	2	0
2	I	1568	1529	1529	9	0
2	K	1626	1587	1587	18	0
3	D	1658	1611	1611	5	0
3	F	1658	1611	1611	7	1
3	J	1650	1607	1607	10	0
3	L	1658	1611	1612	16	0
4	a	125	127	28	0	0
4	g	60	59	14	0	0
5	A	31	11	12	0	0
5	B	31	11	12	0	0
5	G	31	11	12	0	0
5	H	31	12	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	57	0	0	1	0
8	B	85	0	0	1	0
8	C	62	0	0	1	0
8	D	77	0	0	1	0
8	E	52	0	0	1	0
8	F	93	0	0	2	0
8	G	107	0	0	6	0
8	H	85	0	0	6	0
8	I	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	45	0	0	2	0
8	K	61	0	0	3	0
8	L	42	0	0	5	0
All	All	23945	22641	22495	123	1

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 3.

All (123) 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:G:69:LYS:O	1:G:75:ARG:NH1	2.21	0.74
3:J:3:ILE:N	3:J:27:SER:HG	1.91	0.69
1:H:95:LYS:HA	1:H:98:ASN:HB3	1.78	0.66
2:C:139:SER:HA	3:D:119:PHE:HD1	1.60	0.66
3:L:197:CYS:HA	8:L:332:HOH:O	1.97	0.65
2:C:130:VAL:HG21	2:C:207:VAL:HG11	1.77	0.65
2:K:158:PRO:O	8:K:359:HOH:O	2.14	0.64
3:F:126:SER:OG	8:F:301:HOH:O	2.14	0.64
3:L:191:LYS:NZ	8:L:301:HOH:O	2.32	0.62
1:B:224:GLU:OE1	1:B:227:ARG:NH1	2.32	0.62
2:K:209:HIS:ND1	8:K:359:HOH:O	2.31	0.61
3:L:145:ARG:HH11	3:L:145:ARG:HG2	1.64	0.61
3:L:129:LYS:NZ	8:L:323:HOH:O	2.33	0.61
3:L:62:ARG:NH2	3:L:82:GLU:OE1	2.34	0.60
2:K:206:ASN:ND2	2:K:217:ASP:OD1	2.33	0.60
1:H:54:ILE:HG12	1:H:86:MET:HB3	1.83	0.60
1:H:212:ILE:N	8:H:502:HOH:O	2.36	0.59
2:E:157:GLU:OE2	8:E:339:HOH:O	2.17	0.59
3:L:205:SER:O	3:L:206:SER:OG	2.16	0.58
3:D:192:HIS:O	3:D:214:ARG:NH1	2.36	0.58
1:B:339:ASN:ND2	8:B:501:HOH:O	2.36	0.57
3:F:183:THR:OG1	8:F:382:HOH:O	2.17	0.57
3:J:3:ILE:N	3:J:27:SER:OG	2.37	0.56
1:A:169:PRO:HG2	1:B:169:PRO:HG2	1.87	0.56
1:H:54:ILE:HB	8:H:580:HOH:O	2.07	0.55
3:L:151:TRP:HA	8:L:332:HOH:O	2.07	0.55
1:G:311:VAL:O	8:G:589:HOH:O	2.18	0.55
1:G:228:GLN:NE2	8:G:503:HOH:O	2.40	0.55
1:G:159:THR:N	8:G:502:HOH:O	2.36	0.54
1:H:228:GLN:NE2	8:H:503:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:GLU:OE1	3:F:176:TYR:OH	2.24	0.53
3:F:5:MET:SD	3:F:91:GLN:NE2	2.71	0.53
1:G:169:PRO:HG2	1:H:169:PRO:HG2	1.89	0.53
1:H:159:THR:OG1	1:H:160:PHE:N	2.41	0.53
3:J:106:LYS:NZ	8:J:337:HOH:O	2.36	0.53
1:H:9:LEU:HD13	1:H:312:VAL:HG21	1.90	0.53
1:H:81:ASN:ND2	8:H:501:HOH:O	2.32	0.53
1:B:9:LEU:HD13	1:B:312:VAL:HG21	1.91	0.53
2:C:32:LEU:HB2	2:C:37:ILE:HD11	1.90	0.53
1:A:246:PHE:CZ	1:B:322:ARG:HB3	2.44	0.52
2:K:4:GLU:OE1	2:K:4:GLU:N	2.42	0.51
2:K:209:HIS:CE1	2:K:211:PRO:HG2	2.46	0.51
1:G:224:GLU:OE2	1:G:227:ARG:NH2	2.45	0.50
1:H:54:ILE:O	8:H:580:HOH:O	2.20	0.50
2:K:148:GLY:HA2	2:K:163:TRP:CZ2	2.47	0.50
3:F:145:ARG:NH2	3:F:166:VAL:HG21	2.27	0.50
3:D:135:VAL:HG13	3:D:182:LEU:HB3	1.94	0.49
2:C:46:LYS:O	8:C:350:HOH:O	2.20	0.49
2:K:225:CYS:HA	3:L:217:CYS:SG	2.53	0.49
3:L:123:PRO:HD3	3:L:135:VAL:HG22	1.94	0.49
2:C:130:VAL:CG2	2:C:207:VAL:HG11	2.43	0.49
3:L:108:GLU:OE2	3:L:176:TYR:OH	2.31	0.48
3:D:164:GLU:OE2	8:D:371:HOH:O	2.20	0.48
2:K:128:PRO:HB3	2:K:154:TYR:HB3	1.95	0.48
2:K:130:VAL:HG21	2:K:207:VAL:HG11	1.95	0.48
2:C:161:VAL:HG21	2:C:189:SER:HB2	1.96	0.48
2:I:177:ALA:HA	2:I:187:LEU:HB3	1.94	0.48
1:A:317:CYS:HA	1:A:347:ILE:HG23	1.96	0.48
3:J:19:ARG:HG3	3:J:77:SER:HA	1.96	0.47
1:A:81:ASN:N	8:A:521:HOH:O	2.40	0.47
3:D:128:LEU:O	3:D:186:LYS:HD2	2.14	0.47
2:K:172:VAL:O	8:K:341:HOH:O	2.19	0.47
1:A:322:ARG:HB3	1:B:246:PHE:CZ	2.49	0.47
1:H:95:LYS:O	1:H:99:ASP:N	2.45	0.47
1:G:69:LYS:HZ1	2:I:59:SER:CB	2.26	0.47
3:F:30:VAL:HG21	3:F:91:GLN:HB2	1.96	0.47
1:G:284:ASN:O	8:G:579:HOH:O	2.20	0.47
1:B:187:LEU:HD23	1:B:220:LYS:HG2	1.96	0.47
1:G:227:ARG:NH1	8:G:535:HOH:O	2.48	0.47
2:I:130:VAL:HG21	2:I:207:VAL:HG11	1.96	0.47
3:J:111:ARG:HH12	3:J:114:ALA:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:15:VAL:HG21	2:K:21:LEU:HG	1.97	0.47
2:I:209:HIS:HB3	2:I:214:THR:CG2	2.46	0.46
2:I:103:ARG:NH1	2:I:110:ASP:OD2	2.49	0.46
2:K:177:ALA:HA	2:K:187:LEU:HB3	1.98	0.46
3:L:30:VAL:HG21	3:L:91:GLN:HB2	1.97	0.46
1:H:249:LEU:HD11	1:H:298:TYR:CG	2.51	0.46
1:A:246:PHE:CE1	1:A:247:LEU:HD13	2.51	0.45
3:J:103:GLN:NE2	8:J:301:HOH:O	2.48	0.45
2:C:210:LYS:N	2:C:211:PRO:HD2	2.30	0.45
3:L:197:CYS:CA	8:L:332:HOH:O	2.62	0.45
1:H:52:LEU:HD21	1:H:54:ILE:HD11	1.98	0.44
1:G:47:PRO:O	8:G:501:HOH:O	2.21	0.44
3:F:13:SER:HB3	3:F:110:LYS:HB3	1.99	0.44
2:K:210:LYS:N	2:K:211:PRO:HD2	2.33	0.44
3:J:135:VAL:HG13	3:J:182:LEU:HB3	2.00	0.44
2:I:49:GLU:OE1	8:I:311:HOH:O	2.21	0.44
1:A:190:PHE:CE1	1:A:216:LEU:HD23	2.53	0.44
1:B:153:GLU:HG3	1:B:154:GLN:HG3	2.00	0.43
2:K:135:PRO:HD3	2:K:147:LEU:HB3	1.99	0.43
2:I:128:PRO:HD2	2:I:214:THR:HG21	2.00	0.43
1:B:321:ILE:HG22	1:B:327:LEU:HD23	2.00	0.43
3:J:34:VAL:HG21	3:J:72:PHE:CD2	2.54	0.43
1:A:348:TYR:CE1	1:B:286:LYS:HB3	2.53	0.43
1:G:184:SER:OG	1:G:220:LYS:NZ	2.51	0.43
1:H:69:LYS:O	1:H:75:ARG:NH2	2.52	0.43
1:B:265:ASP:OD1	1:B:267:ASN:ND2	2.52	0.43
1:H:98:ASN:HB2	1:H:127:ALA:HB2	2.01	0.42
2:I:15:VAL:HG21	2:I:21:LEU:HB2	2.01	0.42
1:H:165:PHE:HA	8:H:580:HOH:O	2.20	0.42
3:J:38:GLN:HB2	3:J:48:LEU:HD11	2.02	0.42
2:I:210:LYS:N	2:I:211:PRO:HD2	2.35	0.42
2:K:224:SER:O	3:L:217:CYS:SG	2.78	0.42
3:L:166:VAL:HG22	3:L:178:LEU:HD12	2.01	0.42
2:C:110:ASP:OD1	2:C:111:TYR:N	2.53	0.42
3:L:30:VAL:HG23	3:L:93:PRO:HB3	2.02	0.41
1:A:129:LEU:HD21	1:B:185:LYS:HB2	2.02	0.41
1:G:76:LYS:HE2	1:G:81:ASN:O	2.21	0.41
2:K:125:THR:HG21	2:K:211:PRO:O	2.20	0.41
2:K:168:LEU:HD21	2:K:191:VAL:HG11	2.03	0.41
2:C:141:SER:O	2:C:144:THR:OG1	2.35	0.41
2:E:177:ALA:HA	2:E:187:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LEU:HA	1:A:190:PHE:HB3	2.03	0.41
3:J:5:MET:SD	3:J:91:GLN:NE2	2.94	0.41
1:H:321:ILE:HG22	1:H:327:LEU:HD23	2.03	0.41
1:G:9:LEU:HG	1:G:312:VAL:HG21	2.03	0.41
1:A:249:LEU:HD11	1:A:302:ILE:HD11	2.03	0.41
1:G:174:LEU:HD22	1:G:258:GLU:HG2	2.02	0.41
3:L:62:ARG:NH1	3:L:80:GLN:OE1	2.54	0.40
1:A:90:PRO:HG3	1:B:175:ARG:HH21	1.86	0.40
1:G:322:ARG:HB3	1:H:246:PHE:CZ	2.56	0.40
1:B:187:LEU:HB3	1:B:220:LYS:HD3	2.04	0.40
2:K:76:ASP:OD1	2:K:78:SER:OG	2.28	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:210:LYS:NZ	1:G:154:GLN:O[1_645]	2.16	0.04

## 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	295/354 (83%)	287 (97%)	6 (2%)	2 (1%)	26	29
1	B	297/354 (84%)	287 (97%)	9 (3%)	1 (0%)	46	55
1	G	301/354 (85%)	293 (97%)	6 (2%)	2 (1%)	26	29
1	H	303/354 (86%)	288 (95%)	14 (5%)	1 (0%)	46	55
2	C	220/230 (96%)	215 (98%)	5 (2%)	0	100	100
2	E	220/230 (96%)	214 (97%)	6 (3%)	0	100	100
2	I	201/230 (87%)	196 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	K	212/230 (92%)	202 (95%)	9 (4%)	1 (0%)	34	39
3	D	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
3	F	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
3	J	213/217 (98%)	208 (98%)	5 (2%)	0	100	100
3	L	214/217 (99%)	207 (97%)	7 (3%)	0	100	100
All	All	2904/3204 (91%)	2818 (97%)	79 (3%)	7 (0%)	52	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	THR
1	B	170	THR
1	G	170	THR
1	A	285	CYS
1	G	285	CYS
1	H	285	CYS
2	K	135	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	273/309 (88%)	270 (99%)	3 (1%)	80	90
1	B	274/309 (89%)	267 (97%)	7 (3%)	54	68
1	G	275/309 (89%)	270 (98%)	5 (2%)	66	81
1	H	277/309 (90%)	272 (98%)	5 (2%)	66	81
2	C	185/193 (96%)	183 (99%)	2 (1%)	80	90
2	E	185/193 (96%)	183 (99%)	2 (1%)	80	90
2	I	173/193 (90%)	172 (99%)	1 (1%)	90	96
2	K	180/193 (93%)	171 (95%)	9 (5%)	30	37
3	D	191/192 (100%)	190 (100%)	1 (0%)	92	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	191/192 (100%)	189 (99%)	2 (1%)	82	91
3	J	190/192 (99%)	189 (100%)	1 (0%)	92	97
3	L	191/192 (100%)	190 (100%)	1 (0%)	92	97
All	All	2585/2776 (93%)	2546 (98%)	39 (2%)	72	85

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ARG
1	A	227	ARG
1	A	249	LEU
1	B	4	THR
1	B	9	LEU
1	B	88	ILE
1	B	186	LEU
1	B	224	GLU
1	B	279	ASN
1	B	282	GLU
2	C	32	LEU
2	C	206	ASN
3	D	108	GLU
2	E	5	VAL
2	E	206	ASN
3	F	126	SER
3	F	197	CYS
1	G	94	LEU
1	G	211	ASP
1	G	212	ILE
1	G	219	LEU
1	G	266	VAL
1	H	9	LEU
1	H	97	MET
1	H	215	LYS
1	H	222	ASN
1	H	247	LEU
2	I	206	ASN
3	J	202	GLN
2	K	21	LEU
2	K	32	LEU
2	K	125	THR
2	K	161	VAL

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Mol	Chain	Res	Type
2	K	206	ASN
2	K	207	VAL
2	K	209	HIS
2	K	212	SER
2	K	223	LYS
3	L	182	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	310	HIS

### 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 10 ligands modelled in this entry, 6 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	$\# Z  > 2$
5	ATP	A	401	6	24,33,33	2.24	9 (37%)	31,52,52	2.15	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ATP	B	401	6	24,33,33	2.21	8 (33%)	31,52,52	2.27	6 (19%)
5	ATP	G	401	6	24,33,33	2.28	8 (33%)	31,52,52	2.23	7 (22%)
5	ATP	H	401	6	24,33,33	2.24	9 (37%)	31,52,52	2.12	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
5	ATP	A	401	6	-	0/18/38/38	0/3/3/3
5	ATP	B	401	6	-	0/18/38/38	0/3/3/3
5	ATP	G	401	6	-	0/18/38/38	0/3/3/3
5	ATP	H	401	6	-	0/18/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	401	ATP	C2-N1	-5.25	1.23	1.33
5	A	401	ATP	C2-N1	-5.11	1.24	1.33
5	H	401	ATP	C2-N1	-5.02	1.24	1.33
5	B	401	ATP	C2-N1	-4.96	1.24	1.33
5	H	401	ATP	C6-N1	-2.55	1.25	1.37
5	A	401	ATP	C6-N1	-2.55	1.25	1.37
5	B	401	ATP	C6-N1	-2.52	1.25	1.37
5	G	401	ATP	C6-N1	-2.52	1.25	1.37
5	B	401	ATP	C2'-C3'	-2.28	1.47	1.53
5	H	401	ATP	C2'-C3'	-2.19	1.47	1.53
5	A	401	ATP	PG-O2G	-2.12	1.47	1.54
5	H	401	ATP	PG-O2G	-2.09	1.47	1.54
5	A	401	ATP	C2'-C3'	-2.06	1.47	1.53
5	G	401	ATP	C2'-C3'	-2.06	1.47	1.53
5	A	401	ATP	C6-N6	2.75	1.43	1.34
5	H	401	ATP	C6-N6	2.76	1.43	1.34
5	G	401	ATP	C6-N6	2.83	1.43	1.34
5	B	401	ATP	C6-N6	2.89	1.43	1.34
5	H	401	ATP	C5-C4	3.28	1.47	1.40
5	A	401	ATP	C5-C4	3.30	1.47	1.40
5	B	401	ATP	C5-C4	3.38	1.48	1.40
5	G	401	ATP	C5-C4	3.40	1.48	1.40
5	B	401	ATP	C8-N7	3.45	1.41	1.34
5	H	401	ATP	C8-N7	3.46	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	401	ATP	C8-N7	3.58	1.41	1.34
5	A	401	ATP	C8-N7	3.60	1.41	1.34
5	A	401	ATP	C4-N3	3.60	1.40	1.35
5	H	401	ATP	C4-N3	3.91	1.41	1.35
5	B	401	ATP	C4-N3	3.95	1.41	1.35
5	G	401	ATP	C4-N3	4.04	1.41	1.35
5	B	401	ATP	O4'-C1'	4.13	1.46	1.41
5	H	401	ATP	O4'-C1'	4.23	1.46	1.41
5	G	401	ATP	O4'-C1'	4.24	1.46	1.41
5	A	401	ATP	O4'-C1'	4.31	1.46	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	401	ATP	N3-C2-N1	-8.46	122.42	128.89
5	A	401	ATP	N3-C2-N1	-7.99	122.78	128.89
5	H	401	ATP	N3-C2-N1	-7.96	122.80	128.89
5	B	401	ATP	N3-C2-N1	-7.88	122.86	128.89
5	B	401	ATP	PA-O3A-PB	-3.46	123.02	132.73
5	B	401	ATP	PB-O3B-PG	-3.34	121.45	132.67
5	H	401	ATP	PA-O3A-PB	-3.10	124.03	132.73
5	A	401	ATP	PB-O3B-PG	-2.92	122.87	132.67
5	G	401	ATP	PA-O3A-PB	-2.90	124.60	132.73
5	G	401	ATP	PB-O3B-PG	-2.36	124.74	132.67
5	H	401	ATP	PB-O3B-PG	-2.34	124.82	132.67
5	G	401	ATP	O2A-PA-O1A	-2.21	100.54	112.53
5	A	401	ATP	PA-O3A-PB	-2.18	126.60	132.73
5	G	401	ATP	O3G-PG-O1G	-2.09	103.86	110.58
5	H	401	ATP	O3G-PG-O1G	-2.01	104.12	110.58
5	B	401	ATP	O2B-PB-O3A	2.01	114.23	105.09
5	H	401	ATP	O3A-PA-O5'	2.04	108.34	102.94
5	B	401	ATP	O2G-PG-O3B	2.15	114.84	105.09
5	H	401	ATP	O3G-PG-O3B	2.15	114.85	105.09
5	G	401	ATP	O3G-PG-O3B	2.35	115.75	105.09
5	H	401	ATP	C2-N1-C6	5.05	127.78	118.77
5	A	401	ATP	C2-N1-C6	5.22	128.09	118.77
5	G	401	ATP	C2-N1-C6	5.35	128.32	118.77
5	B	401	ATP	C2-N1-C6	5.38	128.39	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/354 (85%)	0.40	18 (5%) 25 38	30, 54, 128, 154	0
1	B	304/354 (85%)	0.30	14 (4%) 36 51	27, 44, 129, 182	0
1	G	307/354 (86%)	0.27	16 (5%) 31 46	27, 43, 111, 166	0
1	H	311/354 (87%)	0.43	23 (7%) 17 27	34, 51, 135, 172	0
2	C	222/230 (96%)	0.24	7 (3%) 51 64	28, 41, 94, 131	0
2	E	222/230 (96%)	0.23	8 (3%) 46 60	28, 43, 84, 151	0
2	I	207/230 (90%)	0.63	30 (14%) 3 6	35, 65, 126, 211	0
2	K	216/230 (93%)	0.96	41 (18%) 2 3	30, 63, 144, 184	0
3	D	216/217 (99%)	0.07	3 (1%) 78 87	28, 47, 73, 114	0
3	F	216/217 (99%)	0.02	1 (0%) 91 96	28, 42, 77, 159	0
3	J	215/217 (99%)	1.15	49 (22%) 1 1	33, 80, 162, 200	0
3	L	216/217 (99%)	0.72	33 (15%) 3 5	31, 60, 141, 175	0
4	a	0/37	-	-	-	-
4	g	0/37	-	-	-	-
All	All	2953/3278 (90%)	0.44	243 (8%) 14 23	27, 49, 132, 211	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	209	THR	10.8
2	K	143	GLY	9.9
3	J	215	GLY	9.4
3	J	211	SER	9.0
1	H	194	THR	8.7
3	J	216	GLU	8.6
3	L	184	LEU	8.3
1	B	190	PHE	7.6
2	I	225	CYS	7.6

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Mol	Chain	Res	Type	RSRZ
2	K	199	GLY	7.3
3	L	157	LEU	7.2
2	I	223	LYS	7.0
2	K	136	SER	6.8
3	J	157	LEU	6.5
2	K	147	LEU	6.4
2	I	203	TYR	6.3
2	K	208	ASN	6.2
2	K	198	LEU	6.1
3	L	129	LYS	6.1
1	G	129	LEU	5.8
1	H	190	PHE	5.7
2	K	193	VAL	5.6
2	E	139	SER	5.6
3	J	154	ASP	5.6
2	I	133	LEU	5.6
1	A	186	LEU	5.2
1	H	195	ASN	5.2
2	C	224	SER	5.1
1	H	186	LEU	5.1
3	J	122	PRO	5.1
2	K	207	VAL	5.1
2	I	168	LEU	5.1
3	L	186	LYS	5.1
3	J	213	ASN	5.1
2	I	136	SER	5.0
3	J	187	ALA	4.9
3	J	195	TYR	4.8
3	J	166	VAL	4.8
3	J	193	LYS	4.8
3	L	193	LYS	4.8
2	I	161	VAL	4.7
2	K	203	TYR	4.6
2	I	147	LEU	4.6
3	J	184	LEU	4.6
1	H	124	GLY	4.6
3	J	155	ASN	4.5
2	K	224	SER	4.5
3	L	132	THR	4.5
1	G	128	ASP	4.5
3	J	150	GLN	4.5
2	I	224	SER	4.5

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Mol	Chain	Res	Type	RSRZ
2	K	134	ALA	4.5
1	H	281	GLN	4.4
1	H	198	GLY	4.4
3	J	191	LYS	4.4
1	H	125	ALA	4.4
1	B	127	ALA	4.3
3	L	128	LEU	4.3
1	B	189	LYS	4.3
1	A	156	GLU	4.3
3	J	25	ARG	4.2
2	I	219	LYS	4.2
2	E	138	LYS	4.2
3	J	199	VAL	4.2
2	E	225	CYS	4.1
2	K	211	PRO	4.1
1	G	281	GLN	4.0
3	L	187	ALA	4.0
1	A	88	ILE	4.0
3	L	190	GLU	3.9
3	J	208	VAL	3.9
3	L	205	SER	3.8
2	K	146	ALA	3.8
2	I	221	GLU	3.8
1	B	280	ASP	3.8
2	K	191	VAL	3.8
3	J	120	ILE	3.8
3	L	185	SER	3.7
3	J	151	TRP	3.7
1	H	98	ASN	3.7
2	I	190	VAL	3.7
2	C	223	LYS	3.7
1	B	155	GLY	3.6
2	K	220	VAL	3.6
1	G	190	PHE	3.5
1	G	197	LEU	3.5
3	J	201	HIS	3.5
3	L	215	GLY	3.4
1	A	155	GLY	3.4
1	B	192	GLU	3.4
1	B	100	MET	3.4
3	L	196	ALA	3.4
3	L	135	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	224	SER	3.4
3	J	153	VAL	3.3
1	H	189	LYS	3.3
1	A	147	LYS	3.3
3	J	148	LYS	3.3
3	J	152	LYS	3.3
2	I	213	ASN	3.3
2	I	195	SER	3.2
3	J	178	LEU	3.2
3	J	156	ALA	3.2
2	K	145	ALA	3.2
3	F	217	CYS	3.2
3	L	182	LEU	3.2
3	J	198	GLU	3.2
1	H	283	HIS	3.1
3	J	192	HIS	3.1
3	J	125	ASP	3.1
2	I	145	ALA	3.1
2	K	225	CYS	3.1
1	B	194	THR	3.1
3	L	189	TYR	3.1
2	E	137	SER	3.0
2	I	14	LEU	3.0
1	H	219	LEU	3.0
2	I	207	VAL	3.0
3	L	125	ASP	2.9
2	I	162	SER	2.9
2	K	214	THR	2.9
1	G	210	VAL	2.9
2	K	183	GLY	2.9
1	H	197	LEU	2.9
3	L	156	ALA	2.9
3	J	118	VAL	2.8
1	B	345	LYS	2.8
1	A	347	ILE	2.8
2	K	196	SER	2.8
3	D	217	CYS	2.8
2	K	194	PRO	2.8
2	K	161	VAL	2.8
3	J	214	ARG	2.8
3	L	195	TYR	2.8
1	G	127	ALA	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	E	200	THR	2.8
1	G	193	ILE	2.8
2	I	134	ALA	2.8
2	C	140	THR	2.8
3	J	212	PHE	2.7
2	I	193	VAL	2.7
1	G	194	THR	2.7
2	C	225	CYS	2.7
2	K	149	CYS	2.7
3	L	154	ASP	2.7
2	K	209	HIS	2.7
2	K	223	LYS	2.7
3	L	155	ASN	2.7
3	L	152	LYS	2.6
1	G	159	THR	2.6
1	A	128	ASP	2.6
2	K	5	VAL	2.6
2	K	150	LEU	2.6
2	I	204	ILE	2.6
3	J	200	THR	2.6
3	J	189	TYR	2.6
2	E	141	SER	2.5
3	J	206	SER	2.5
1	H	126	LEU	2.5
3	L	206	SER	2.5
2	I	167	ALA	2.5
3	J	138	LEU	2.5
3	L	212	PHE	2.5
1	G	285	CYS	2.5
1	H	284	ASN	2.5
2	K	154	TYR	2.5
2	K	212	SER	2.5
3	L	160	GLY	2.5
1	B	148	HIS	2.5
1	G	352	ASP	2.5
2	I	172	VAL	2.5
2	I	194	PRO	2.5
3	J	149	VAL	2.5
2	I	220	VAL	2.5
1	A	150	LYS	2.4
3	L	153	VAL	2.4
1	G	284	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	136	SER	2.4
1	H	214	GLY	2.4
1	H	143	MET	2.4
3	L	2	ASP	2.4
1	A	103	SER	2.4
2	K	169	THR	2.4
3	L	122	PRO	2.3
3	L	183	THR	2.3
3	J	145	ARG	2.3
3	J	95	TYR	2.3
1	A	129	LEU	2.3
2	K	181	SER	2.3
3	L	134	SER	2.3
2	K	159	VAL	2.3
2	K	135	PRO	2.3
3	J	136	VAL	2.3
3	L	123	PRO	2.3
2	K	201	GLN	2.3
1	H	285	CYS	2.3
1	A	351	GLU	2.3
2	K	148	GLY	2.3
1	H	246	PHE	2.3
2	C	219	LYS	2.3
3	J	144	PRO	2.2
3	D	129	LYS	2.2
1	A	279	ASN	2.2
1	A	130	THR	2.2
2	K	162	SER	2.2
3	L	194	VAL	2.2
3	J	123	PRO	2.2
1	B	193	ILE	2.2
2	K	200	THR	2.2
1	A	189	LYS	2.2
2	C	200	THR	2.2
2	K	202	THR	2.2
3	J	77	SER	2.2
3	D	187	ALA	2.2
2	I	222	PRO	2.2
3	J	133	ALA	2.2
1	B	150	LYS	2.1
1	H	212	ILE	2.1
3	J	109	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	178	VAL	2.1
1	H	154	GLN	2.1
3	J	139	LEU	2.1
2	C	201	GLN	2.1
3	J	196	ALA	2.1
2	I	164	ASN	2.1
1	G	211	ASP	2.1
1	B	281	GLN	2.1
1	A	215	LYS	2.1
1	A	325	ASN	2.1
2	I	146	ALA	2.1
1	A	153	GLU	2.1
1	G	95	LYS	2.1
1	B	285	CYS	2.0
2	K	144	THR	2.0
1	A	152	GLN	2.0
2	K	170	SER	2.0
2	K	92	GLU	2.0
1	H	280	ASP	2.0
2	I	175	PHE	2.0
1	H	127	ALA	2.0
1	G	351	GLU	2.0
3	L	211	SER	2.0
3	J	217	CYS	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
6	MG	B	402	1/1	0.97	0.14	1.78	35,35,35,35	0
5	ATP	B	401	31/31	0.97	0.14	0.38	25,34,41,43	0
5	ATP	A	401	31/31	0.98	0.13	0.17	32,39,46,48	0
5	ATP	G	401	31/31	0.97	0.14	0.05	36,43,60,68	0
5	ATP	H	401	31/31	0.97	0.14	-0.09	35,38,46,47	0
7	ZN	G	403	1/1	0.99	0.15	-0.18	56,56,56,56	0
6	MG	H	402	1/1	0.98	0.13	-0.41	37,37,37,37	0
7	ZN	A	403	1/1	0.97	0.14	-0.45	55,55,55,55	0
6	MG	G	402	1/1	0.99	0.10	-1.48	42,42,42,42	0
6	MG	A	402	1/1	0.98	0.10	-2.48	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.