



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:02 PM GMT

PDB ID : 4GSK  
Title : Crystal structure of an Atg7-Atg10 crosslinked complex  
Authors : Kaiser, S.E.; Mao, K.; Taherbhoy, A.M.; Yu, S.; Olszewski, J.L.; Duda, D.M.;  
Kurinov, I.; Deng, A.; Fenn, T.D.; Klionsky, D.J.; Schulman, B.A.  
Deposited on : 2012-08-27  
Resolution : 2.90 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

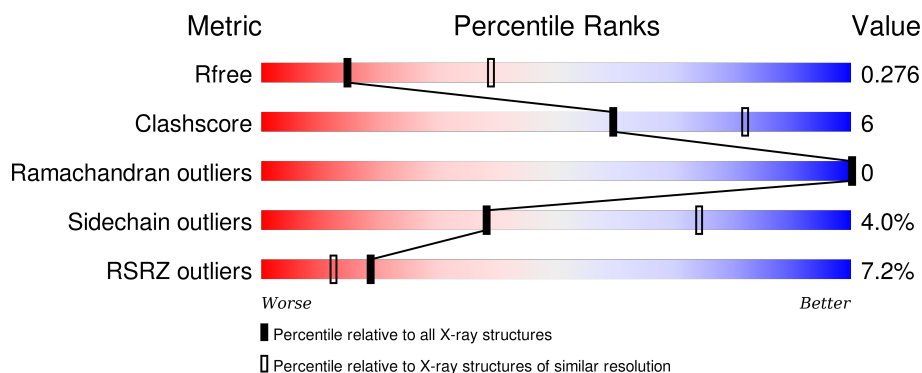
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	615	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	615	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
2	Y	173	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>12%</div> <div>• 21%</div> </div> </div>
2	Z	173	<div> <div>5%</div> <div> <div></div> <div>60%</div> <div>14%</div> <div>• 24%</div> </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
3	ZN	A	701	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11408 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 Ubiquitin-like modifier-activating enzyme ATG7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	570	Total	C	N	O	S	0	0	0
			4548	2930	768	829	21			
1	B	572	Total	C	N	O	S	0	0	0
			4573	2946	774	832	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P38862
A	0	SER	-	EXPRESSION TAG	UNP P38862
A	39	SER	CYS	ENGINEERED MUTATION	UNP P38862
A	195	SER	CYS	ENGINEERED MUTATION	UNP P38862
A	375	ALA	CYS	ENGINEERED MUTATION	UNP P38862
B	-1	GLY	-	EXPRESSION TAG	UNP P38862
B	0	SER	-	EXPRESSION TAG	UNP P38862
B	39	SER	CYS	ENGINEERED MUTATION	UNP P38862
B	195	SER	CYS	ENGINEERED MUTATION	UNP P38862
B	375	ALA	CYS	ENGINEERED MUTATION	UNP P38862

- Molecule 2 is a protein called Ubiquitin-like-conjugating enzyme ATG10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	137	Total	C	N	O	S	0	0	0
			1161	758	190	210	3			
2	Z	131	Total	C	N	O	S	0	0	0
			1124	737	184	200	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-5	GLY	-	EXPRESSION TAG	UNP Q07879
Y	-4	SER	-	EXPRESSION TAG	UNP Q07879

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Chain	Residue	Modelled	Actual	Comment	Reference
Y	-3	GLY	-	EXPRESSION TAG	UNP Q07879
Y	-2	GLY	-	EXPRESSION TAG	UNP Q07879
Y	-1	SER	-	EXPRESSION TAG	UNP Q07879
Y	0	GLY	-	EXPRESSION TAG	UNP Q07879
Y	26	SER	CYS	ENGINEERED MUTATION	UNP Q07879
Y	137	SER	CYS	ENGINEERED MUTATION	UNP Q07879
Z	-5	GLY	-	EXPRESSION TAG	UNP Q07879
Z	-4	SER	-	EXPRESSION TAG	UNP Q07879
Z	-3	GLY	-	EXPRESSION TAG	UNP Q07879
Z	-2	GLY	-	EXPRESSION TAG	UNP Q07879
Z	-1	SER	-	EXPRESSION TAG	UNP Q07879
Z	0	GLY	-	EXPRESSION TAG	UNP Q07879
Z	26	SER	CYS	ENGINEERED MUTATION	UNP Q07879
Z	137	SER	CYS	ENGINEERED MUTATION	UNP Q07879

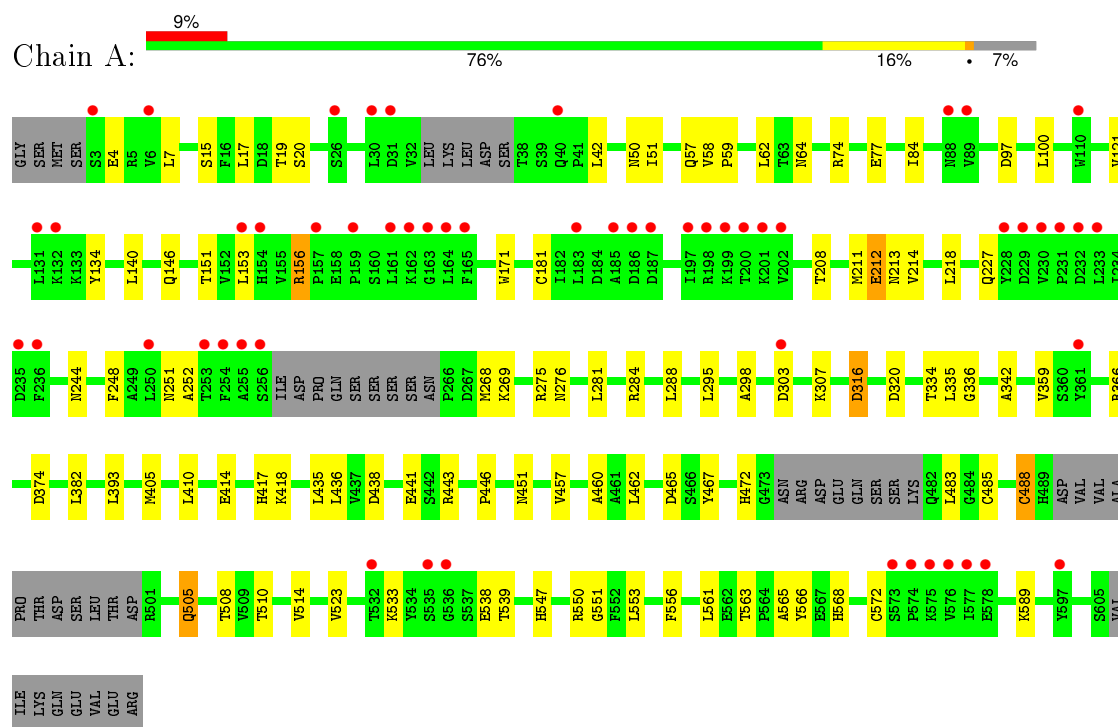
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

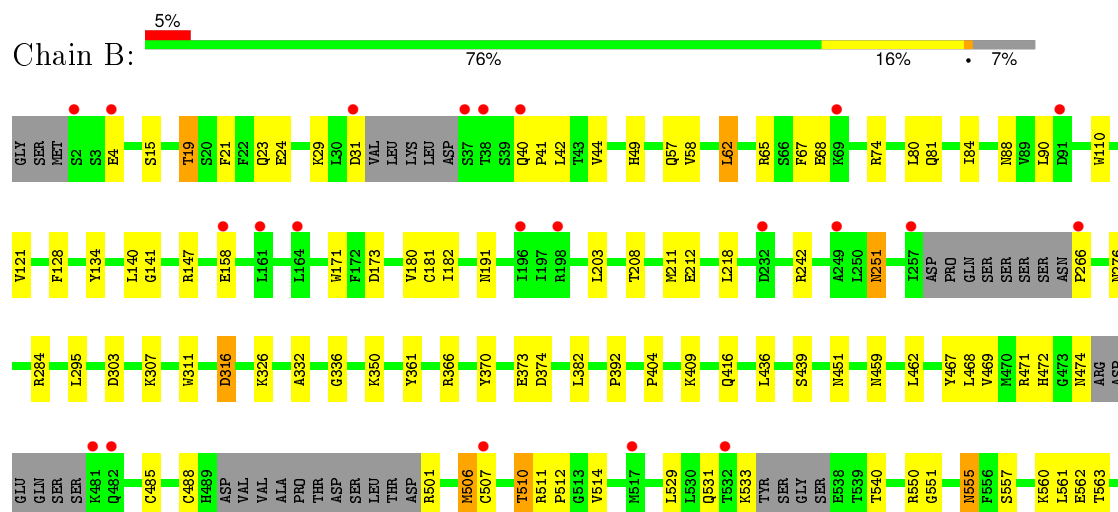
### 3 Residue-property plots

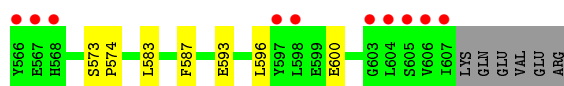
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Ubiquitin-like modifier-activating enzyme ATG7

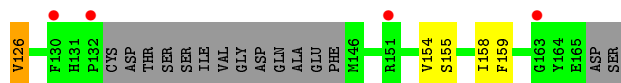


- Molecule 1: Ubiquitin-like modifier-activating enzyme ATG7

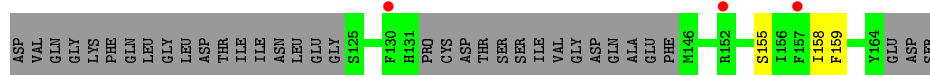
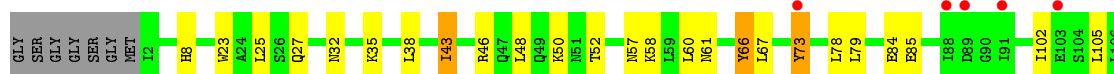




● Molecule 2: Ubiquitin-like-conjugating enzyme ATG10



● Molecule 2: Ubiquitin-like-conjugating enzyme ATG10



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.56 Å 146.19 Å 108.44 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.90 49.57 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.56-2.90) 92.4 (49.57-2.90)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.91 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1000)	Depositor
R, $R_{free}$	0.236 , 0.285 0.227 , 0.276	Depositor DCC
$R_{free}$ test set	2007 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.3	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	1 of 42709 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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

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	0.26	0/4646	0.45	0/6291
1	B	0.26	0/4669	0.46	0/6318
2	Y	0.25	0/1193	0.45	0/1621
2	Z	0.26	0/1155	0.44	0/1568
All	All	0.26	0/11663	0.45	0/15798

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	4548	0	4604	52	0
1	B	4573	0	4648	49	0
2	Y	1161	0	1139	14	0
2	Z	1124	0	1114	18	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	11408	0	11505	130	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (130) 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)
2:Y:49:GLN:HE22	2:Y:60:LEU:H	1.19	0.89
1:A:15:SER:HB3	1:A:140:LEU:HD22	1.59	0.84
2:Y:81:ARG:HH21	2:Y:126:VAL:HB	1.56	0.70
1:B:15:SER:HB3	1:B:140:LEU:HD22	1.77	0.66
2:Z:61:ASN:HD22	2:Z:85:GLU:HG2	1.62	0.64
1:B:307:LYS:HE2	1:B:311:TRP:HE1	1.62	0.64
1:B:462:LEU:HD22	1:B:514:VAL:HG12	1.80	0.62
1:A:462:LEU:HD22	1:A:514:VAL:HG12	1.82	0.61
1:B:295:LEU:HD21	1:B:392:PRO:HB2	1.82	0.61
1:B:409:LYS:HA	1:B:593:GLU:HG2	1.82	0.61
1:B:374:ASP:HB3	1:B:382:LEU:HD21	1.82	0.61
1:A:212:GLU:HG2	1:A:213:ASN:HD22	1.64	0.61
2:Z:27:GLN:HE21	2:Z:43:ILE:HG13	1.66	0.60
2:Z:155:SER:HA	2:Z:159:PHE:HB2	1.84	0.59
1:B:58:VAL:HG12	1:B:208:THR:HB	1.85	0.59
1:A:457:VAL:HB	1:A:472:HIS:HB2	1.84	0.59
1:B:276:ASN:HA	1:B:284:ARG:HE	1.68	0.59
2:Z:67:LEU:HD21	2:Z:158:ILE:HD11	1.83	0.58
1:A:467:TYR:CZ	1:A:551:GLY:HA3	2.39	0.58
1:A:20:SER:HB2	1:A:64:ASN:HD22	1.68	0.57
1:A:472:HIS:CE1	1:A:485:CYS:HB2	2.38	0.57
1:A:533:LYS:NZ	1:A:538:GLU:OE1	2.33	0.57
2:Y:8:HIS:CE1	2:Y:35:LYS:HB2	2.39	0.57
1:A:435:LEU:HD21	1:A:446:PRO:HB2	1.86	0.57
1:A:211:MET:HB3	1:A:214:VAL:HB	1.89	0.55
1:B:439:SER:HB3	1:B:506:MET:HB2	1.88	0.55
1:B:121:VAL:HG22	1:B:218:LEU:HD22	1.89	0.54
1:A:298:ALA:HB2	1:B:361:TYR:HB3	1.89	0.53
2:Y:52:THR:HG21	2:Y:60:LEU:HD13	1.90	0.53
2:Y:155:SER:HA	2:Y:159:PHE:HB2	1.90	0.53
2:Y:3:PRO:HG2	2:Y:6:GLU:HB2	1.89	0.53
1:A:58:VAL:HG12	1:A:208:THR:HB	1.88	0.53
2:Y:65:LEU:HD22	2:Y:78:LEU:HD11	1.90	0.53
1:B:467:TYR:CZ	1:B:551:GLY:HA3	2.44	0.52
2:Y:49:GLN:NE2	2:Y:60:LEU:H	1.98	0.52
1:B:326:LYS:HG2	1:B:350:LYS:HD3	1.91	0.52
1:A:335:LEU:HD21	1:A:462:LEU:HD21	1.91	0.52
2:Z:48:LEU:O	2:Z:52:THR:HG23	2.09	0.51
2:Z:58:LYS:HD3	2:Z:84:GLU:CD	2.31	0.51
1:B:555:ASN:ND2	1:B:557:SER:OG	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:LEU:HB2	1:B:587:PHE:HB2	1.94	0.50
1:A:97:ASP:OD1	1:A:100:LEU:N	2.39	0.50
2:Y:67:LEU:HD21	2:Y:158:ILE:HD11	1.92	0.50
1:A:295:LEU:HD11	1:A:393:LEU:HG	1.93	0.50
1:A:374:ASP:HB3	1:A:382:LEU:HD21	1.94	0.49
1:B:171:TRP:CZ3	1:B:181:CYS:HB3	2.47	0.49
2:Y:52:THR:HG21	2:Y:60:LEU:HD22	1.94	0.49
1:B:507:CYS:HB3	2:Z:73:TYR:CE1	2.48	0.49
1:A:443:ARG:NH2	1:A:460:ALA:O	2.39	0.49
1:B:21:PHE:CE1	1:B:62:LEU:HD12	2.47	0.49
1:A:121:VAL:HG22	1:A:218:LEU:HD22	1.94	0.48
1:A:336:GLY:HA2	1:A:436:LEU:HD13	1.95	0.48
1:A:505:GLN:O	1:A:508:THR:HG22	2.14	0.48
1:A:483:LEU:HB3	1:A:547:HIS:CD2	2.49	0.48
1:B:468:LEU:HD13	1:B:550:ARG:HG2	1.96	0.47
1:B:65:ARG:NH1	1:B:68:GLU:OE1	2.34	0.47
1:B:29:LYS:HE3	1:B:88:ASN:HD22	1.78	0.47
1:A:156:ARG:HG2	1:A:251:ASN:HB3	1.97	0.47
1:A:405:MET:HE2	1:A:441:GLU:HG3	1.97	0.46
1:B:212:GLU:OE1	1:B:212:GLU:N	2.45	0.46
1:A:414:GLU:O	1:A:418:LYS:HG2	2.15	0.46
1:A:334:THR:HG23	1:A:366:ARG:O	2.16	0.46
2:Y:67:LEU:HD23	2:Y:78:LEU:HD13	1.97	0.46
1:B:471:ARG:HD2	1:B:529:LEU:HD21	1.98	0.46
1:A:465:ASP:HB2	1:A:553:LEU:HB2	1.97	0.45
1:A:276:ASN:HA	1:A:284:ARG:HE	1.81	0.45
1:A:316:ASP:N	1:A:316:ASP:OD1	2.50	0.45
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.80	0.45
1:B:49:HIS:HE1	1:B:173:ASP:OD1	2.00	0.45
1:B:44:VAL:HG13	1:B:80:LEU:HB3	1.99	0.45
2:Z:35:LYS:HA	2:Z:35:LYS:HD3	1.71	0.45
2:Z:46:ARG:O	2:Z:50:LYS:HG2	2.16	0.44
1:B:472:HIS:CE1	1:B:485:CYS:HB2	2.52	0.44
2:Z:8:HIS:HE1	2:Z:35:LYS:HB2	1.81	0.44
1:A:342:ALA:HB3	1:A:523:VAL:HG21	1.98	0.44
1:B:140:LEU:HG	1:B:141:GLY:N	2.32	0.44
2:Z:38:LEU:HD23	2:Z:67:LEU:HD12	2.00	0.44
1:A:550:ARG:HE	1:A:550:ARG:HB2	1.64	0.44
1:A:7:LEU:HD22	1:A:153:LEU:HD23	1.99	0.44
2:Z:60:LEU:HA	2:Z:60:LEU:HD12	1.87	0.44
1:A:153:LEU:HD11	1:A:252:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:HG2	1:B:67:PHE:CD1	2.52	0.44
1:B:211:MET:O	1:B:242:ARG:NH2	2.34	0.44
2:Y:23:TRP:CZ2	2:Y:25:LEU:HD12	2.52	0.43
2:Z:23:TRP:CZ2	2:Z:25:LEU:HD12	2.53	0.43
1:A:556:PHE:HB2	1:B:560:LYS:HD3	1.99	0.43
1:B:110:TRP:CH2	1:B:147:ARG:HD2	2.54	0.43
1:B:182:ILE:HG22	1:B:203:LEU:HD12	2.01	0.43
1:A:359:VAL:HG21	1:A:382:LEU:HD23	2.01	0.42
1:B:42:LEU:HD11	1:B:84:ILE:HB	1.99	0.42
1:B:158:GLU:OE1	1:B:251:ASN:ND2	2.51	0.42
1:B:40:GLN:HA	1:B:41:PRO:HD3	1.87	0.42
1:B:90:LEU:HB2	1:B:128:PHE:CE2	2.55	0.42
1:A:303:ASP:O	1:A:307:LYS:HG2	2.18	0.42
1:A:42:LEU:HD11	1:A:84:ILE:HB	2.01	0.42
1:A:213:ASN:HA	1:A:248:PHE:CZ	2.54	0.42
1:A:410:LEU:HD11	1:A:589:LYS:HG3	2.02	0.42
1:A:74:ARG:HB2	1:A:77:GLU:HG3	2.01	0.42
2:Y:80:LEU:HD12	2:Y:81:ARG:H	1.85	0.41
1:B:303:ASP:O	1:B:307:LYS:HG2	2.20	0.41
1:A:366:ARG:NH2	1:A:510:THR:O	2.51	0.41
1:A:171:TRP:CZ3	1:A:181:CYS:HB3	2.55	0.41
1:B:316:ASP:N	1:B:316:ASP:OD1	2.52	0.41
1:A:268:MET:HE3	1:A:268:MET:HB2	1.95	0.41
1:B:531:GLN:HB2	1:B:540:THR:HB	2.02	0.41
1:B:511:ARG:HA	1:B:512:PRO:HD3	1.90	0.41
1:A:275:ARG:HG2	1:A:281:LEU:HD23	2.01	0.41
2:Z:66:TYR:HB3	2:Z:79:LEU:HB2	2.02	0.41
2:Z:32:ASN:OD1	2:Z:32:ASN:N	2.54	0.41
1:A:566:TYR:CE2	1:A:568:HIS:HB2	2.56	0.41
1:B:332:ALA:HB1	1:B:370:TYR:OH	2.19	0.41
1:B:562:GLU:HG2	1:B:563:THR:H	1.86	0.41
1:B:404:PRO:HB3	1:B:416:GLN:NE2	2.35	0.41
1:A:51:ILE:HG23	1:A:59:PRO:HD3	2.03	0.41
1:B:459:ASN:O	1:B:469:VAL:HA	2.20	0.41
1:A:488:CYS:SG	1:A:565:ALA:HA	2.61	0.41
1:A:17:LEU:HD22	1:A:62:LEU:HB2	2.02	0.41
1:B:336:GLY:HA2	1:B:436:LEU:HD13	2.03	0.41
1:B:366:ARG:NH1	1:B:510:THR:O	2.36	0.41
2:Y:154:VAL:HG13	2:Y:158:ILE:HD12	2.03	0.40
2:Z:52:THR:HA	2:Z:105:LEU:HD11	2.03	0.40
1:A:550:ARG:HH21	1:A:561:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:OE1	1:A:269:LYS:HE2	2.22	0.40
2:Z:67:LEU:HD23	2:Z:78:LEU:HD13	2.03	0.40
2:Z:52:THR:HG21	2:Z:60:LEU:HD22	2.03	0.40
1:A:151:THR:HG21	1:A:227:GLN:HE22	1.87	0.40
1:B:19:THR:O	1:B:23:GLN:HG2	2.22	0.40
1:B:147:ARG:HH11	1:B:266:PRO:HD2	1.87	0.40
1:A:17:LEU:HD22	1:A:62:LEU:HD12	2.02	0.40
1:B:573:SER:HA	1:B:574:PRO:HD3	1.92	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	560/615 (91%)	549 (98%)	11 (2%)	0	100	100
1	B	560/615 (91%)	550 (98%)	10 (2%)	0	100	100
2	Y	131/173 (76%)	125 (95%)	6 (5%)	0	100	100
2	Z	125/173 (72%)	121 (97%)	4 (3%)	0	100	100
All	All	1376/1576 (87%)	1345 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	510/555 (92%)	492 (96%)	18 (4%)	43	78
1	B	515/555 (93%)	491 (95%)	24 (5%)	32	68
2	Y	130/160 (81%)	126 (97%)	4 (3%)	47	82
2	Z	127/160 (79%)	122 (96%)	5 (4%)	39	75
All	All	1282/1430 (90%)	1231 (96%)	51 (4%)	38	74

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	19	THR
1	A	50	ASN
1	A	57	GLN
1	A	134	TYR
1	A	156	ARG
1	A	212	GLU
1	A	244	ASN
1	A	316	ASP
1	A	320	ASP
1	A	417	HIS
1	A	438	ASP
1	A	451	ASN
1	A	488	CYS
1	A	505	GLN
1	A	539	THR
1	A	563	THR
1	A	572	CYS
1	B	4	GLU
1	B	19	THR
1	B	31	ASP
1	B	57	GLN
1	B	62	LEU
1	B	74	ARG
1	B	81	GLN
1	B	134	TYR
1	B	180	VAL
1	B	191	ASN
1	B	251	ASN
1	B	316	ASP
1	B	373	GLU
1	B	451	ASN
1	B	474	ASN

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Mol	Chain	Res	Type
1	B	488	CYS
1	B	501	ARG
1	B	506	MET
1	B	510	THR
1	B	533	LYS
1	B	555	ASN
1	B	561	LEU
1	B	596	LEU
1	B	600	GLU
2	Y	57	ASN
2	Y	66	TYR
2	Y	106	LEU
2	Y	126	VAL
2	Z	43	ILE
2	Z	57	ASN
2	Z	66	TYR
2	Z	73	TYR
2	Z	102	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	50	ASN
1	A	64	ASN
1	A	213	ASN
1	A	489	HIS
1	B	49	HIS
1	B	81	GLN
1	B	86	ASN
1	B	88	ASN
1	B	104	GLN
1	B	278	GLN
1	B	408	HIS
1	B	416	GLN
1	B	417	HIS
1	B	474	ASN
1	B	505	GLN
1	B	548	GLN
1	B	555	ASN
2	Y	5	GLN
2	Y	49	GLN

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Mol	Chain	Res	Type
2	Y	61	ASN
2	Z	8	HIS
2	Z	21	HIS
2	Z	27	GLN
2	Z	61	ASN

### 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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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	570/615 (92%)	0.68	55 (9%) 10 6	61, 80, 97, 105	0
1	B	572/615 (93%)	0.55	32 (5%) 28 21	60, 76, 94, 104	0
2	Y	137/173 (79%)	0.51	7 (5%) 32 25	66, 83, 96, 103	0
2	Z	131/173 (75%)	0.54	8 (6%) 25 18	68, 79, 93, 100	0
All	All	1410/1576 (89%)	0.60	102 (7%) 18 12	60, 78, 96, 105	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	SER	6.1
1	B	481	LYS	5.3
1	B	38	THR	5.2
1	A	597	TYR	4.7
1	A	255	ALA	4.5
1	B	607	ILE	4.1
1	A	232	ASP	4.1
1	A	201	LYS	4.1
1	A	199	LYS	3.9
2	Y	132	PRO	3.8
2	Z	73	TYR	3.8
1	B	2	SER	3.8
1	B	604	LEU	3.8
1	A	163	GLY	3.7
1	A	183	LEU	3.7
1	A	6	VAL	3.7
1	B	606	VAL	3.7
1	A	202	VAL	3.7
1	A	233	LEU	3.6
1	B	257	ILE	3.6
1	A	236	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	40	GLN	3.5
1	A	132	LYS	3.5
1	A	574	PRO	3.5
1	B	566	TYR	3.5
1	A	254	PHE	3.4
1	B	507	CYS	3.4
1	B	91	ASP	3.3
1	A	131	LEU	3.3
1	A	536	GLY	3.3
2	Y	88	ILE	3.2
1	A	200	THR	3.2
1	B	31	ASP	3.2
1	A	110	TRP	3.1
1	A	235	ASP	3.0
1	B	568	HIS	3.0
1	A	256	SER	3.0
1	A	186	ASP	3.0
1	A	159	PRO	3.0
1	B	482	GLN	3.0
2	Z	88	ILE	3.0
1	A	535	SER	3.0
1	A	578	GLU	2.9
1	A	303	ASP	2.9
1	A	157	PRO	2.9
1	B	161	LEU	2.9
1	A	162	LYS	2.9
1	A	575	LYS	2.8
1	A	198	ARG	2.8
1	A	361	TYR	2.7
1	B	232	ASP	2.7
2	Z	152	ARG	2.7
1	A	230	VAL	2.7
1	A	576	VAL	2.7
2	Z	91	ILE	2.7
1	A	161	LEU	2.7
1	B	40	GLN	2.6
1	A	187	ASP	2.6
1	A	30	LEU	2.6
1	B	598	LEU	2.6
1	B	605	SER	2.6
2	Y	130	PHE	2.6
1	A	228	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	250	LEU	2.5
1	A	185	ALA	2.5
2	Z	89	ASP	2.5
1	A	31	ASP	2.5
1	A	3	SER	2.4
2	Y	151	ARG	2.4
1	B	266	PRO	2.4
1	B	597	TYR	2.4
1	A	577	ILE	2.4
1	B	196	ILE	2.4
2	Y	89	ASP	2.4
1	B	517	MET	2.4
1	A	89	VAL	2.4
1	A	88	ASN	2.3
1	A	165	PHE	2.3
1	A	229	ASP	2.3
1	B	198	ARG	2.3
1	A	26	SER	2.3
1	B	69	LYS	2.3
2	Y	125	SER	2.3
1	A	231	PRO	2.3
1	B	164	LEU	2.2
1	A	253	THR	2.2
1	A	532	THR	2.2
1	B	532	THR	2.2
1	B	249	ALA	2.2
2	Y	163	GLY	2.2
1	B	158	GLU	2.2
2	Z	157	PHE	2.2
1	A	154	HIS	2.2
1	B	567	GLU	2.1
2	Z	130	PHE	2.1
1	A	153	LEU	2.1
1	A	197	ILE	2.1
1	B	4	GLU	2.1
1	A	573	SER	2.1
2	Z	103	GLU	2.1
1	B	603	GLY	2.0
1	A	164	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( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	701	1/1	0.98	0.28	2.65	88,88,88,88	0
3	ZN	B	701	1/1	0.91	0.21	-0.31	92,92,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.