Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2023 – 07:09 PM EDT

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

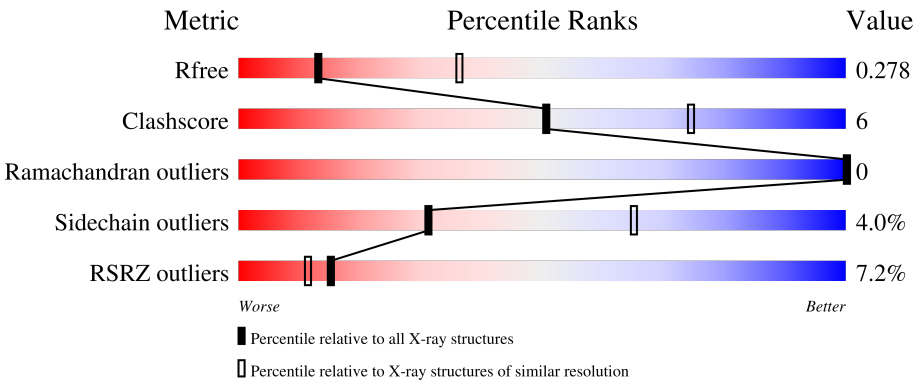
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	9% 76% 16% • 7%
1	B	615	5% 76% 16% • 7%
2	Y	173	4% 66% 12% • 21%
2	Z	173	5% 60% 14% • 24%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	570	4548	2930	768	829	21	0	0	0
1	B	572	4573	2946	774	832	21	0	0	0

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
			Total	C	N	O	S			
2	Y	137	1161	758	190	210	3	0	0	0
2	Z	131	1124	737	184	200	3	0	0	0

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).

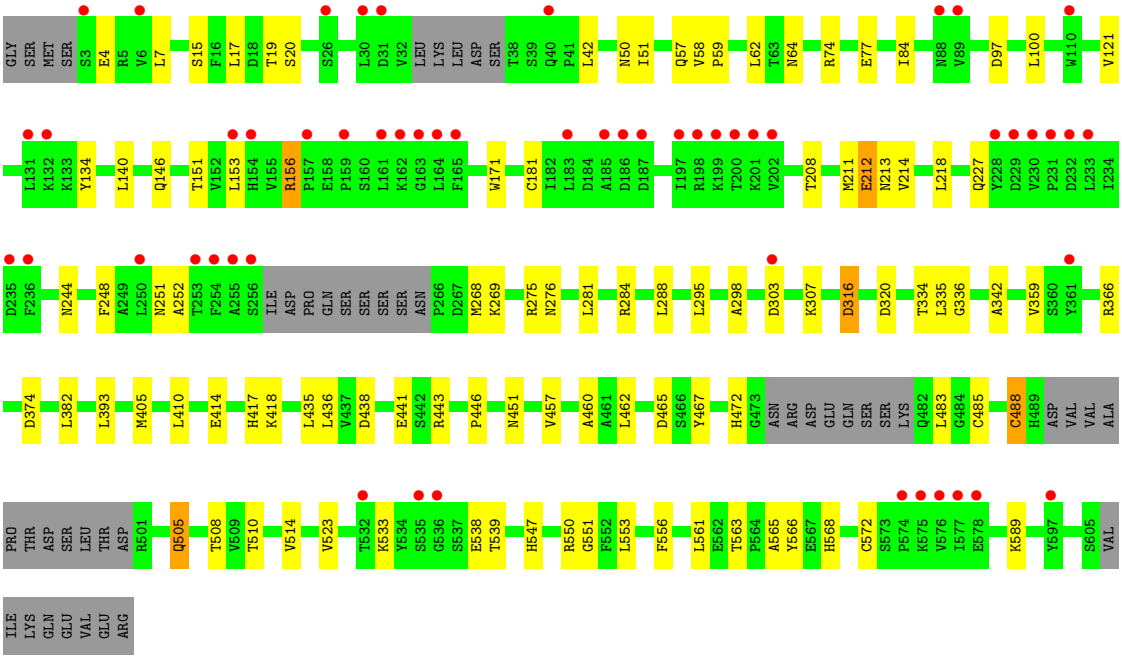
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

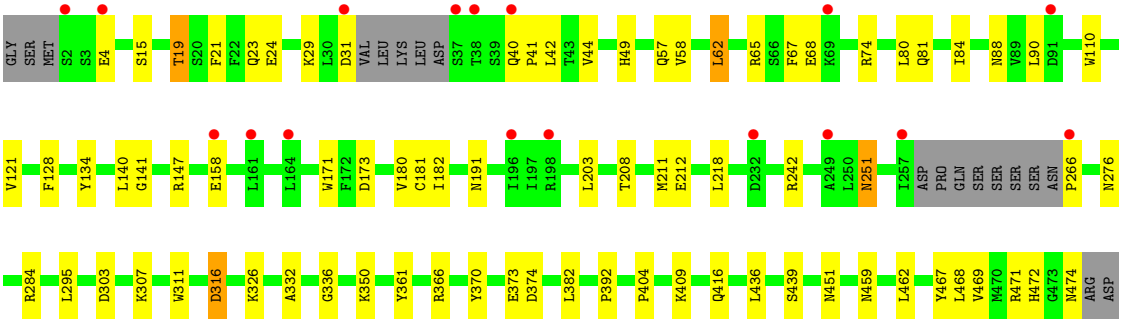
• Molecule 1: Ubiquitin-like modifier-activating enzyme ATG7

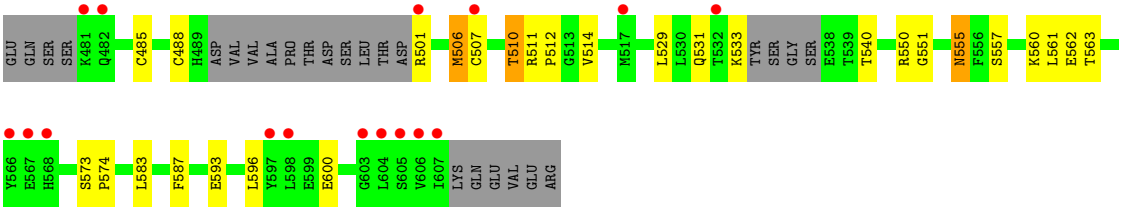
Chain A:



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

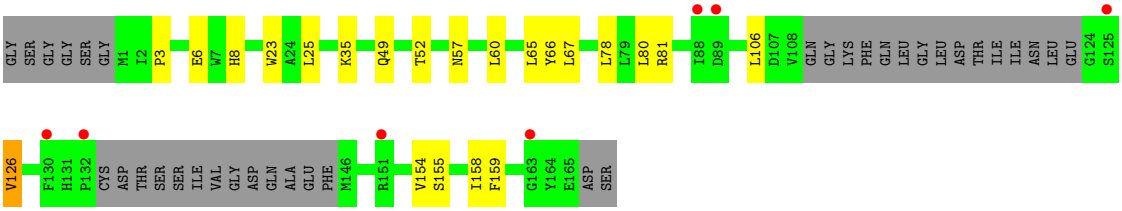
Chain B:





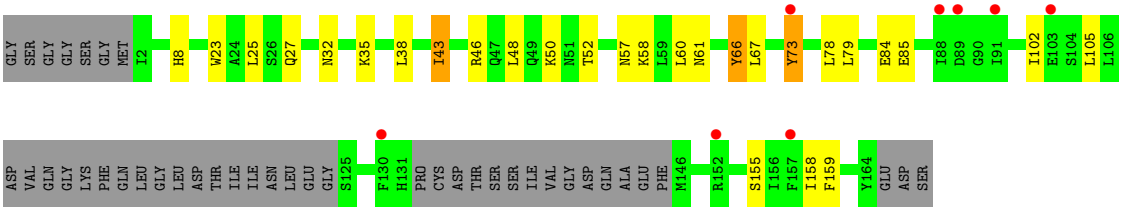
- Molecule 2: Ubiquitin-like-conjugating enzyme ATG10

Chain Y:



- Molecule 2: Ubiquitin-like-conjugating enzyme ATG10

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	120.56Å 146.19Å 108.44Å 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
$< I/\sigma(I) >$ [1]	1.92 (at 2.91Å)	Xtriage
Refinement program	PHENIX dev_1000	Depositor
R, R_{free}	0.236 , 0.285 0.230 , 0.278	Depositor DCC
R_{free} test set	2154 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 53.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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 (i)

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:374:ASP:HB3	1:B:382:LEU:HD21	1.82	0.61
1:B:409:LYS:HA	1:B:593:GLU:HG2	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
1:A:58:VAL:HG12	1:A:208:THR:HB	1.88	0.53
2:Y:3:PRO:HG2	2:Y:6:GLU:HB2	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: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:29:LYS:HE3	1:B:88:ASN:HD22	1.78	0.47
1:B:65:ARG:NH1	1:B:68:GLU:OE1	2.34	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:A:334:THR:HG23	1:A:366:ARG:O	2.16	0.46
1:A:414:GLU:O	1:A:418:LYS:HG2	2.15	0.46
1:B:212:GLU:OE1	1:B:212:GLU:N	2.45	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:276:ASN:HA	1:A:284:ARG:HE	1.81	0.45
1:A:465:ASP:HB2	1:A:553:LEU:HB2	1.97	0.45
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.80	0.45
1:A:316:ASP:OD1	1:A:316:ASP:N	2.50	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
1:B:472:HIS:CE1	1:B:485:CYS:HB2	2.52	0.44
2:Z:46:ARG:O	2:Z:50:LYS:HG2	2.16	0.44
1:A:342:ALA:HB3	1:A:523:VAL:HG21	1.98	0.44
2:Z:8:HIS:HE1	2:Z:35:LYS:HB2	1.81	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:7:LEU:HD22	1:A:153:LEU:HD23	1.99	0.44
1:A:550:ARG:HE	1:A:550:ARG:HB2	1.64	0.44
2:Z:60:LEU:HD12	2:Z:60:LEU:HA	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:40:GLN:HA	1:B:41:PRO:HD3	1.87	0.42
1:B:158:GLU:OE1	1:B:251:ASN:ND2	2.51	0.42
1:A:303:ASP:O	1:A:307:LYS:HG2	2.18	0.42
1:B:90:LEU:HB2	1:B:128:PHE:CE2	2.55	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:74:ARG:HB2	1:A:77:GLU:HG3	2.01	0.42
1:A:410:LEU:HD11	1:A:589:LYS:HG3	2.02	0.42
1:A:171:TRP:CZ3	1:A:181:CYS:HB3	2.55	0.41
1:A:366:ARG:NH2	1:A:510:THR:O	2.51	0.41
1:B:303:ASP:O	1:B:307:LYS:HG2	2.20	0.41
2:Y:80:LEU:HD12	2:Y:81:ARG:H	1.85	0.41
1:B:316:ASP:OD1	1:B:316:ASP:N	2.52	0.41
1:A:268:MET:HB2	1:A:268:MET:HE3	1.95	0.41
1:B:531:GLN:HB2	1:B:540:THR:HB	2.02	0.41
1:A:275:ARG:HG2	1:A:281:LEU:HD23	2.01	0.41
1:B:511:ARG:HA	1:B:512:PRO:HD3	1.90	0.41
2:Z:66:TYR:HB3	2:Z:79:LEU:HB2	2.02	0.41
1:A:566:TYR:CE2	1:A:568:HIS:HB2	2.56	0.41
2:Z:32:ASN:OD1	2:Z:32:ASN:N	2.54	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:A:17:LEU:HD22	1:A:62:LEU:HB2	2.02	0.41
1:A:51:ILE:HG23	1:A:59:PRO:HD3	2.03	0.41
1:A:488:CYS:SG	1:A:565:ALA:HA	2.61	0.41
1:B:336:GLY:HA2	1:B:436:LEU:HD13	2.03	0.41
1:B:404:PRO:HB3	1:B:416:GLN:NE2	2.35	0.41
1:B:459:ASN:O	1:B:469:VAL:HA	2.20	0.41
1:B:366:ARG:NH1	1:B:510:THR:O	2.36	0.41
1:A:550:ARG:HH21	1:A:561:LEU:HD21	1.86	0.40
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

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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
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
2:Z:52:THR:HG21	2:Z:60:LEU:HD22	2.03	0.40
2:Z:67:LEU:HD23	2:Z:78:LEU:HD13	2.03	0.40
1:A:17:LEU:HD22	1:A:62:LEU:HD12	2.02	0.40
1:B:147:ARG:HH11	1:B:266:PRO:HD2	1.87	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%)	36	70
1	B	515/555 (93%)	491 (95%)	24 (5%)	26	59
2	Y	130/160 (81%)	126 (97%)	4 (3%)	40	74
2	Z	127/160 (79%)	122 (96%)	5 (4%)	32	66
All	All	1282/1430 (90%)	1231 (96%)	51 (4%)	31	65

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

Sometimes 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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	570/615 (92%)	0.66	54 (9%)	8	6	61, 80, 97, 105	0
1	B	572/615 (93%)	0.53	33 (5%)	23	19	60, 76, 94, 104	0
2	Y	137/173 (79%)	0.49	7 (5%)	28	24	66, 83, 96, 103	0
2	Z	131/173 (75%)	0.52	8 (6%)	21	17	68, 79, 93, 100	0
All	All	1410/1576 (89%)	0.58	102 (7%)	15	11	60, 78, 96, 105	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	SER	6.0
1	B	481	LYS	5.2
1	B	38	THR	5.1
1	A	255	ALA	4.6
1	A	597	TYR	4.5
1	B	607	ILE	4.1
1	A	201	LYS	4.0
1	A	232	ASP	3.9
1	A	199	LYS	3.8
2	Z	73	TYR	3.7
1	B	2	SER	3.7
1	A	183	LEU	3.7
2	Y	132	PRO	3.7
1	A	163	GLY	3.7
1	A	202	VAL	3.7
1	B	604	LEU	3.7
1	B	606	VAL	3.7
1	A	6	VAL	3.6
1	A	233	LEU	3.5
1	B	257	ILE	3.5
1	A	236	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	132	LYS	3.4
1	A	40	GLN	3.4
1	B	566	TYR	3.4
1	A	574	PRO	3.4
1	A	254	PHE	3.4
1	B	507	CYS	3.3
1	A	536	GLY	3.2
1	A	131	LEU	3.2
1	B	91	ASP	3.2
2	Y	88	ILE	3.2
1	A	200	THR	3.1
1	B	31	ASP	3.1
1	B	568	HIS	3.0
1	A	110	TRP	3.0
1	A	198	ARG	2.9
1	A	256	SER	2.9
1	A	235	ASP	2.9
1	A	159	PRO	2.9
1	A	535	SER	2.9
1	B	482	GLN	2.9
1	A	186	ASP	2.9
2	Z	88	ILE	2.9
1	B	161	LEU	2.9
2	Z	152	ARG	2.8
1	A	303	ASP	2.8
1	A	162	LYS	2.8
1	A	578	GLU	2.8
1	A	157	PRO	2.8
1	A	575	LYS	2.8
1	A	576	VAL	2.7
1	A	361	TYR	2.7
1	A	230	VAL	2.7
2	Z	91	ILE	2.7
1	A	161	LEU	2.7
1	B	232	ASP	2.6
1	B	598	LEU	2.6
1	A	30	LEU	2.6
1	B	40	GLN	2.6
2	Y	130	PHE	2.6
2	Y	151	ARG	2.6
1	B	605	SER	2.5
1	A	185	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	187	ASP	2.5
1	A	250	LEU	2.5
1	A	228	TYR	2.5
1	A	577	ILE	2.4
1	B	196	ILE	2.4
1	B	597	TYR	2.4
1	A	3	SER	2.4
2	Z	89	ASP	2.4
1	B	198	ARG	2.4
1	A	31	ASP	2.4
1	A	89	VAL	2.3
1	B	266	PRO	2.3
1	B	517	MET	2.3
2	Y	89	ASP	2.3
1	A	165	PHE	2.3
1	B	69	LYS	2.2
1	B	249	ALA	2.2
1	A	88	ASN	2.2
1	A	26	SER	2.2
1	A	229	ASP	2.2
2	Y	163	GLY	2.2
1	B	164	LEU	2.2
2	Y	125	SER	2.2
1	B	532	THR	2.2
1	A	231	PRO	2.2
1	A	532	THR	2.2
2	Z	157	PHE	2.1
1	A	154	HIS	2.1
1	A	253	THR	2.1
2	Z	130	PHE	2.1
1	B	158	GLU	2.1
1	A	153	LEU	2.1
1	B	501	ARG	2.1
1	B	567	GLU	2.1
1	A	197	ILE	2.0
1	B	603	GLY	2.0
1	A	164	LEU	2.0
1	B	4	GLU	2.0
2	Z	103	GLU	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	ZN	B	701	1/1	0.91	0.21	92,92,92,92	0
3	ZN	A	701	1/1	0.98	0.28	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.