

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	8J09
Title	:	Crystal structure of protein 3745
Authors	:	Li, H.; Yao, M.
Deposited on	:	2023-04-10
Resolution	:	2.61 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
	·	4.020-401
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.61 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	А	267	5%	17%	• 10%			
2	В	650	3% 68%	16% •	15%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6516 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 DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	241	Total 1983	C 1286	N 332	O 359	S 6	0	0	0

• Molecule 2 is a protein called Cell division control protein 45.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	555	Total 4493	C 2876	N 754	0 849	S 14	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	16	Total O 16 16	0	0
3	В	24	Total O 24 24	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: DNA replication regulator SLD3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	70.77Å 107.57Å 128.28Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	43.47 - 2.61	Depositor
Resolution (A)	43.47 - 2.61	EDS
% Data completeness	99.9 (43.47-2.61)	Depositor
(in resolution range)	99.9(43.47-2.61)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.05 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
P. P.	0.219 , 0.262	Depositor
n, n_{free}	0.219 , 0.262	DCC
R_{free} test set	1570 reflections (5.13%)	wwPDB-VP
Wilson B-factor $(Å^2)$	43.9	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31 , 45.3	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	0.93	EDS
Total number of atoms	6516	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/2018	0.40	0/2713	
2	В	0.25	0/4578	0.45	1/6199~(0.0%)	
All	All	0.25	0/6596	0.43	1/8912~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	538	LEU	CA-CB-CG	5.75	128.52	115.30

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	А	1983	0	2061	25	0
2	В	4493	0	4489	74	0
3	А	16	0	0	0	0
3	В	24	0	0	0	0
All	All	6516	0	6550	99	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 8.

All (99) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:16:LEU:HD21	2:B:52:GLN:HE22	1.47	0.80	
2:B:506:ILE:HG13	2:B:547:ARG:HD3	1.67	0.73	
2:B:526:ARG:NH1	2:B:558:GLU:OE2	2.22	0.71	
2:B:312:THR:HG22	2:B:314:ASP:H	1.56	0.70	
2:B:537:ASP:O	2:B:539:TYR:N	2.26	0.68	
2:B:31:VAL:HG22	2:B:42:THR:HG21	1.78	0.66	
2:B:231:HIS:O	2:B:231:HIS:ND1	2.25	0.65	
2:B:19:SER:HA	2:B:26:GLN:HG3	1.77	0.65	
2:B:556:CYS:SG	2:B:563:GLN:NE2	2.73	0.62	
2:B:537:ASP:C	2:B:539:TYR:H	2.02	0.61	
2:B:282:ILE:HD12	2:B:283:ALA:N	2.18	0.58	
2:B:546:LEU:HD11	2:B:629:ILE:HD11	1.84	0.58	
2:B:249:ASN:ND2	2:B:250:SER:H	2.01	0.58	
1:A:228:LEU:HD22	1:A:244:LEU:HD21	1.86	0.57	
2:B:249:ASN:HD22	2:B:250:SER:H	1.52	0.57	
2:B:531:GLN:HA	2:B:572:ILE:HG22	1.87	0.56	
2:B:633:ARG:NH1	2:B:635:GLU:OE2	2.39	0.56	
2:B:344:VAL:HG12	2:B:401:LEU:HD22	1.87	0.55	
1:A:357:LEU:HD11	1:A:378:LYS:HE2	1.89	0.55	
2:B:1:MET:N	2:B:137:SER:O	2.32	0.55	
1:A:206:ALA:O	1:A:210:LYS:HG2	2.07	0.54	
2:B:463:ALA:O	2:B:464:GLN:HG3	2.08	0.54	
2:B:311:LYS:O	2:B:312:THR:OG1	2.25	0.54	
2:B:267:LEU:HB3	2:B:316:LEU:HD22	1.88	0.54	
2:B:399:TYR:HB2	2:B:401:LEU:HD12	1.90	0.53	
2:B:101:GLN:HA	2:B:104:VAL:HG23	1.90	0.53	
1:A:271:ILE:HG21	1:A:350:ALA:HB2	1.89	0.52	
2:B:354:ASN:O	2:B:358:ARG:HG3	2.09	0.52	
2:B:382:HIS:HA	2:B:385:LYS:HD3	1.92	0.51	
2:B:386:ARG:HG2	2:B:386:ARG:NH1	2.25	0.51	
1:A:360:GLU:O	1:A:361:THR:HG22	2.10	0.51	
2:B:531:GLN:O	2:B:533:GLY:N	2.44	0.51	
1:A:258:THR:HG23	1:A:374:ILE:HG21	1.94	0.49	
2:B:538:LEU:HD21	2:B:573:ASP:HA	1.94	0.49	
1:A:204:TYR:CZ	1:A:208:LEU:HD11	2.47	0.49	
2:B:158:ALA:HB1	2:B:233:TYR:HB3	1.95	0.49	
2:B:561:ASP:OD2	2:B:561:ASP:N	2.46	0.49	
2:B:410:VAL:HG13	2:B:418:SER:HB2	1.95	0.49	
2:B:610:GLN:HB2	2:B:627:SER:HB3	1.94	0.48	
2:B:325:TYR:HB3	2:B:404:ILE:HA	1.95	0.48	
2:B:353:GLU:O	2:B:357:LYS:HG3	2.14	0.48	
2:B:357:LYS:O	2:B:361:LYS:HG3	2.14	0.48	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:379:LYS:N	1:A:379:LYS:HD3	2.28	0.48
2:B:90:ILE:O	2:B:133:ASN:ND2	2.46	0.48
2:B:16:LEU:HD21	2:B:52:GLN:NE2	2.24	0.47
1:A:157:PRO:HA	1:A:160:TYR:HB3	1.94	0.47
2:B:633:ARG:HB3	2:B:635:GLU:OE2	2.15	0.47
1:A:390:LEU:HB3	1:A:417:LEU:HD13	1.95	0.46
2:B:564:LEU:HD22	2:B:600:PRO:HD3	1.98	0.46
2:B:587:ARG:HD3	2:B:587:ARG:HA	1.62	0.45
2:B:356:LYS:HE2	2:B:360:HIS:CE1	2.51	0.45
2:B:464:GLN:O	2:B:467:THR:OG1	2.19	0.45
2:B:610:GLN:HB2	2:B:627:SER:CB	2.46	0.45
1:A:205:GLN:HB2	1:A:284:LEU:HD13	1.99	0.45
2:B:52:GLN:O	2:B:54:VAL:N	2.50	0.45
2:B:553:ILE:HG23	2:B:563:GLN:OE1	2.17	0.45
2:B:325:TYR:CZ	2:B:590:ARG:HB3	2.52	0.45
1:A:337:LEU:HG	1:A:338:ASP:N	2.31	0.44
1:A:179:PHE:HD1	1:A:183:ASN:HD22	1.66	0.44
1:A:248:VAL:HG21	1:A:259:ILE:HD11	1.99	0.44
2:B:538:LEU:O	2:B:538:LEU:HD23	2.16	0.44
2:B:598:LYS:HE3	2:B:598:LYS:HB3	1.84	0.44
2:B:386:ARG:HG2	2:B:386:ARG:HH11	1.80	0.44
1:A:254:LYS:HE3	1:A:254:LYS:HB2	1.78	0.44
2:B:604:ASN:HB2	2:B:607:MET:HE3	1.99	0.44
2:B:161:LYS:HG3	2:B:233:TYR:CE2	2.52	0.43
1:A:207:MET:HE2	1:A:207:MET:HB2	1.83	0.43
2:B:479:LEU:HD22	2:B:491:LEU:HD21	2.00	0.43
1:A:375:GLN:O	1:A:378:LYS:N	2.50	0.43
2:B:163:LEU:HD23	2:B:163:LEU:H	1.84	0.43
2:B:351:TRP:HB3	2:B:511:VAL:HG22	2.01	0.43
2:B:521:HIS:CE1	2:B:562:LYS:HD3	2.53	0.43
2:B:595:ILE:C	2:B:597:THR:H	2.22	0.43
2:B:16:LEU:O	2:B:20:SER:OG	2.26	0.43
1:A:406:VAL:HG13	1:A:406:VAL:O	2.17	0.43
2:B:15:ILE:HD13	2:B:82:LEU:HD11	1.99	0.43
2:B:537:ASP:C	2:B:539:TYR:N	2.72	0.43
1:A:163:SER:O	1:A:167:ASP:HB2	2.19	0.43
2:B:45:LEU:HD21	2:B:255:ILE:HD12	2.00	0.43
2:B:526:ARG:NH2	2:B:563:GLN:OE1	2.41	0.43
2:B:572:ILE:HB	2:B:579:TYR:CE1	2.54	0.43
1:A:237:ASP:OD1	1:A:240:ARG:NE	2.41	0.42
1:A:361:THR:O	1:A:362:PRO:C	2.57	0.42

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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:381:ASP:HB3	2:B:384:ILE:HD12	2.01	0.42
2:B:435:GLY:O	2:B:494:ARG:NH1	2.52	0.42
1:A:248:VAL:HG13	1:A:249:ILE:HG13	2.01	0.42
2:B:360:HIS:CE1	2:B:370:LEU:HD21	2.55	0.42
2:B:535:ASP:OD1	2:B:536:LEU:N	2.51	0.42
2:B:128:PRO:HB2	2:B:240:TYR:CZ	2.55	0.42
2:B:635:GLU:H	2:B:635:GLU:CD	2.24	0.41
1:A:386:LYS:O	1:A:392:GLY:HA3	2.20	0.41
2:B:573:ASP:O	2:B:577:ASP:N	2.52	0.41
1:A:222:HIS:CE1	1:A:267:LYS:HA	2.56	0.41
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.92	0.41
2:B:228:LYS:HB3	2:B:229:GLN:H	1.77	0.41
2:B:282:ILE:HD12	2:B:283:ALA:H	1.86	0.41
2:B:388:LEU:HD23	2:B:388:LEU:HA	1.87	0.41
2:B:436:ASN:ND2	2:B:475:SER:OG	2.51	0.41
2:B:517:LYS:HA	2:B:517:LYS:HD3	1.91	0.40

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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	Perce	ntiles
1	А	235/267~(88%)	225~(96%)	6 (3%)	4 (2%)	9	16
2	В	545/650~(84%)	509 (93%)	30 (6%)	6 (1%)	14	27
All	All	780/917~(85%)	734 (94%)	36~(5%)	10 (1%)	12	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	361	THR
1	А	362	PRO
	~	-	



COULU	Continucu from previous page						
Mol	Chain	Res	Type				
2	В	53	LEU				
2	В	532	ASP				
2	В	537	ASP				
2	В	538	LEU				
2	В	464	GLN				
1	А	155	SER				
2	В	627	SER				
1	А	315	VAL				

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5.3.2Protein 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	А	225/249~(90%)	217~(96%)	8 (4%)	35 59
2	В	499/586~(85%)	486~(97%)	13 (3%)	46 70
All	All	724/835~(87%)	703~(97%)	21 (3%)	42 67

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	167	ASP
1	А	186	ARG
1	А	253	ASN
1	А	268	SER
1	А	292	ARG
1	А	337	LEU
1	А	371	ASN
1	А	384	LYS
2	В	22	HIS
2	В	51	LYS
2	В	163	LEU
2	В	164	GLU
2	В	231	HIS
2	В	249	ASN
2	В	311	LYS



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Mol	Chain	Res	Type
2	В	353	GLU
2	В	416	ARG
2	В	462	SER
2	В	475	SER
2	В	540	ARG
2	В	602	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
2	В	52	GLN
2	В	57	GLN
2	В	249	ASN
2	В	321	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	А	241/267~(90%)	0.06	14 (5%) 23 18	26, 49, 101, 125	0
2	В	555/650~(85%)	0.13	22 (3%) 38 32	27, 52, 89, 121	0
All	All	796/917~(86%)	0.11	36 (4%) 33 27	26, 51, 93, 125	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	536	LEU	5.2
1	А	315	VAL	4.9
1	А	253	ASN	4.8
1	А	362	PRO	4.3
2	В	461	ASN	4.2
1	А	252	GLU	4.1
1	А	370	SER	4.0
1	А	314	LEU	3.9
2	В	539	TYR	3.8
2	В	164	GLU	3.6
2	В	538	LEU	3.6
2	В	462	SER	3.5
2	В	114	GLN	3.4
2	В	533	GLY	3.2
2	В	51	LYS	3.2
2	В	437	SER	2.9
2	В	628	SER	2.8
2	В	53	LEU	2.7
2	В	463	ALA	2.6
1	А	371	ASN	2.6
2	В	165	LEU	2.6
1	А	316	ARG	2.4
2	В	354	ASN	2.4
2	В	316	LEU	2.4



Mol	Chain	Res	Type	RSRZ
2	В	534	PRO	2.2
2	В	535	ASP	2.2
1	А	256	SER	2.2
1	А	419	GLY	2.2
1	А	251	ASP	2.1
1	А	254	LYS	2.1
2	В	416	ARG	2.1
2	В	561	ASP	2.1
1	А	155	SER	2.1
2	В	304	PRO	2.0
2	В	379	TYR	2.0
1	А	248	VAL	2.0

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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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

