



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 18, 2024 – 04:33 PM JST

PDB ID : 8J09
Title : Crystal structure of the Sld3 Cdc45-binding-domain, in complex with Cdc45
Authors : Li, H.; Ishizaka, I.; Kato, K.; Sun, X.; Muramatsu, S.; Itou, H.; Ose, T.; Araki, 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

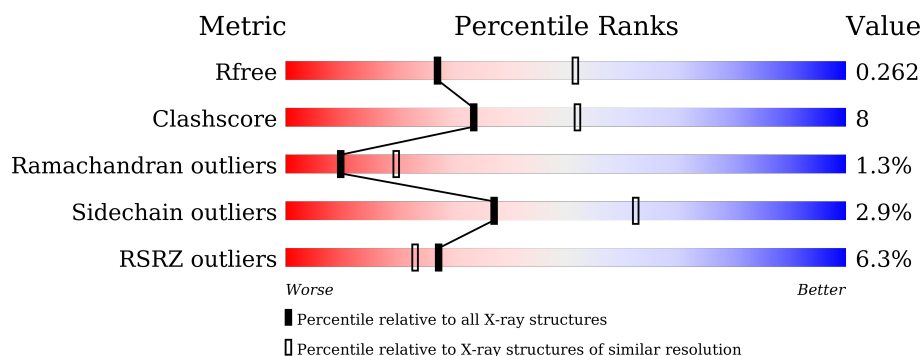
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (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 $\leq 5\%$. 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	267	
2	B	650	

2 Entry composition

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	A	241	Total	C	N	O	S	0	0	0
			1983	1286	332	359	6			

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

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

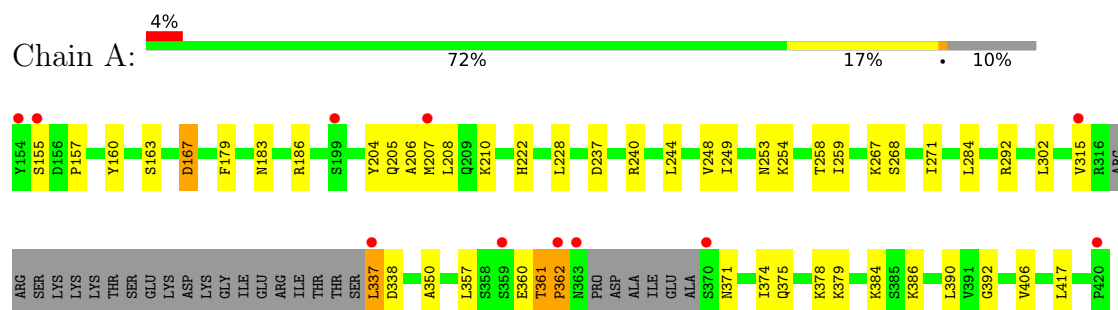
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	24	Total	O	0	0
			24	24		

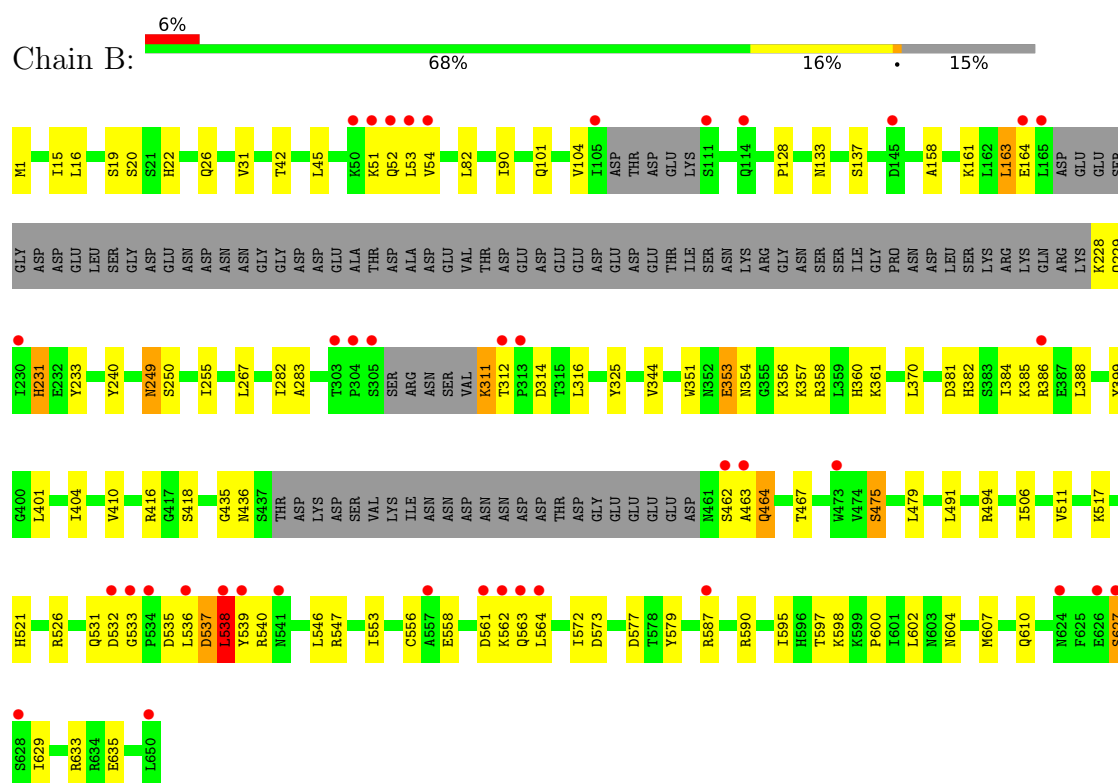
3 Residue-property plots [i](#)

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



• Molecule 2: Cell division control protein 45



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.77Å 107.57Å 128.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.47 – 2.61 43.47 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.9 (43.47-2.61) 99.9 (43.47-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.219 , 0.262 0.219 , 0.262	Depositor DCC
R_{free} test set	1562 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)	0.32 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/2018	0.40	0/2713
2	B	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(°)	Ideal(°)
2	B	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	A	1983	0	2061	25	0
2	B	4493	0	4489	74	0
3	A	16	0	0	0	0
3	B	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 distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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 distance (Å)	Clash 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

There are no symmetry-related clashes.

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	235/267 (88%)	225 (96%)	6 (3%)	4 (2%)	7	14
2	B	545/650 (84%)	509 (93%)	30 (6%)	6 (1%)	12	24
All	All	780/917 (85%)	734 (94%)	36 (5%)	10 (1%)	10	20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	THR
1	A	362	PRO

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Mol	Chain	Res	Type
2	B	53	LEU
2	B	532	ASP
2	B	537	ASP
2	B	538	LEU
2	B	464	GLN
1	A	155	SER
2	B	627	SER
1	A	315	VAL

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	225/249 (90%)	217 (96%)	8 (4%)	30	54
2	B	499/586 (85%)	486 (97%)	13 (3%)	41	66
All	All	724/835 (87%)	703 (97%)	21 (3%)	37	62

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

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

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

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

Mol	Chain	Res	Type
2	B	52	GLN
2	B	57	GLN
2	B	249	ASN
2	B	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 oligosaccharides 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

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, 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	241/267 (90%)	0.11	11 (4%) 38 33	26, 49, 101, 125	0
2	B	555/650 (85%)	0.26	39 (7%) 24 20	27, 52, 89, 121	0
All	All	796/917 (86%)	0.21	50 (6%) 27 23	26, 51, 93, 125	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	536	LEU	5.3
2	B	539	TYR	4.8
2	B	538	LEU	4.1
2	B	53	LEU	3.9
2	B	51	LYS	3.9
2	B	628	SER	3.7
1	A	370	SER	3.6
1	A	337	LEU	3.4
2	B	304	PRO	3.2
1	A	315	VAL	3.1
2	B	557	ALA	3.1
1	A	362	PRO	3.1
2	B	533	GLY	3.1
2	B	305	SER	3.0
2	B	230	ILE	2.9
2	B	312	THR	2.9
2	B	650	LEU	2.8
2	B	563	GLN	2.8
1	A	154	TYR	2.7
1	A	363	ASN	2.7
2	B	463	ALA	2.7
2	B	303	THR	2.6
2	B	561	ASP	2.6
2	B	111	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	114	GLN	2.5
2	B	624	ASN	2.5
2	B	626	GLU	2.5
2	B	462	SER	2.4
2	B	587	ARG	2.4
2	B	50	LYS	2.4
2	B	165	LEU	2.3
2	B	54	VAL	2.3
2	B	473	TRP	2.3
1	A	207	MET	2.3
2	B	562	LYS	2.3
2	B	145	ASP	2.2
2	B	105	ILE	2.2
2	B	541	ASN	2.2
2	B	52	GLN	2.2
2	B	386	ARG	2.2
2	B	564	LEU	2.2
1	A	420	PRO	2.1
2	B	164	GLU	2.1
2	B	534	PRO	2.1
2	B	627	SER	2.1
1	A	199	SER	2.1
2	B	313	PRO	2.1
1	A	155	SER	2.1
1	A	359	SER	2.0
2	B	532	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.