



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

PDB ID : 3RTR
Title : A RING E3-substrate complex poised for ubiquitin-like protein transfer: structural insights into cullin-RING ligases
Authors : Calabrese, M.F.; Scott, D.C.; Duda, D.M.; Grace, C.R.; Kurinov, I.; Kriwacki, R.W.; Schulman, B.A.
Deposited on : 2011-05-03
Resolution : 3.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

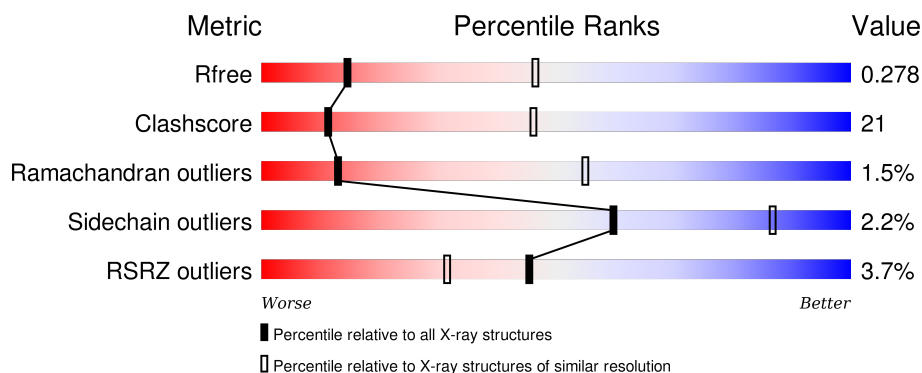
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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 ≥ 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	368	<div> <div>2%</div> <div>55%</div> <div>39%</div> <div>• •</div> </div>
1	C	368	<div> <div>5%</div> <div>45%</div> <div>39%</div> <div>• 14%</div> </div>
1	E	368	<div> <div>4%</div> <div>57%</div> <div>38%</div> <div>• •</div> </div>
1	G	368	<div> <div>3%</div> <div>57%</div> <div>39%</div> <div>• •</div> </div>
2	B	106	<div> <div>4%</div> <div>52%</div> <div>29%</div> <div>19%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	106	<div><div>%</div><div><div></div><div>45%</div><div>29%</div><div>25%</div></div></div>
2	F	106	<div><div>%</div><div><div></div><div>47%</div><div>29%</div><div>24%</div></div></div>
2	H	106	<div><div>4%</div><div><div></div><div>40%</div><div>35%</div><div>•</div><div>24%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14055 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 Cullin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	0	0
			2870	1822	485	549	14			
1	C	317	Total	C	N	O	S	0	0	0
			2592	1647	439	494	12			
1	E	359	Total	C	N	O	S	0	0	0
			2918	1853	492	560	13			
1	G	360	Total	C	N	O	S	0	0	0
			2937	1866	495	562	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	GLY	-	EXPRESSION TAG	UNP Q13616
A	410	SER	-	EXPRESSION TAG	UNP Q13616
A	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616
A	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
A	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
A	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616
C	409	GLY	-	EXPRESSION TAG	UNP Q13616
C	410	SER	-	EXPRESSION TAG	UNP Q13616
C	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616
C	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
C	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
C	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616
E	409	GLY	-	EXPRESSION TAG	UNP Q13616
E	410	SER	-	EXPRESSION TAG	UNP Q13616
E	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616
E	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
E	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
E	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616
G	409	GLY	-	EXPRESSION TAG	UNP Q13616
G	410	SER	-	EXPRESSION TAG	UNP Q13616
G	421	GLU	LEU	ENGINEERED MUTATION	UNP Q13616

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Chain	Residue	Modelled	Actual	Comment	Reference
G	451	GLU	VAL	ENGINEERED MUTATION	UNP Q13616
G	452	LYS	VAL	ENGINEERED MUTATION	UNP Q13616
G	455	LYS	TYR	ENGINEERED MUTATION	UNP Q13616

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			713	452	129	123	9			
2	D	79	Total	C	N	O	S	0	0	0
			658	419	119	111	9			
2	F	81	Total	C	N	O	S	0	0	0
			684	436	124	115	9			
2	H	81	Total	C	N	O	S	0	0	0
			671	427	121	114	9			

There are 8 discrepancies between the modelled and reference sequences:

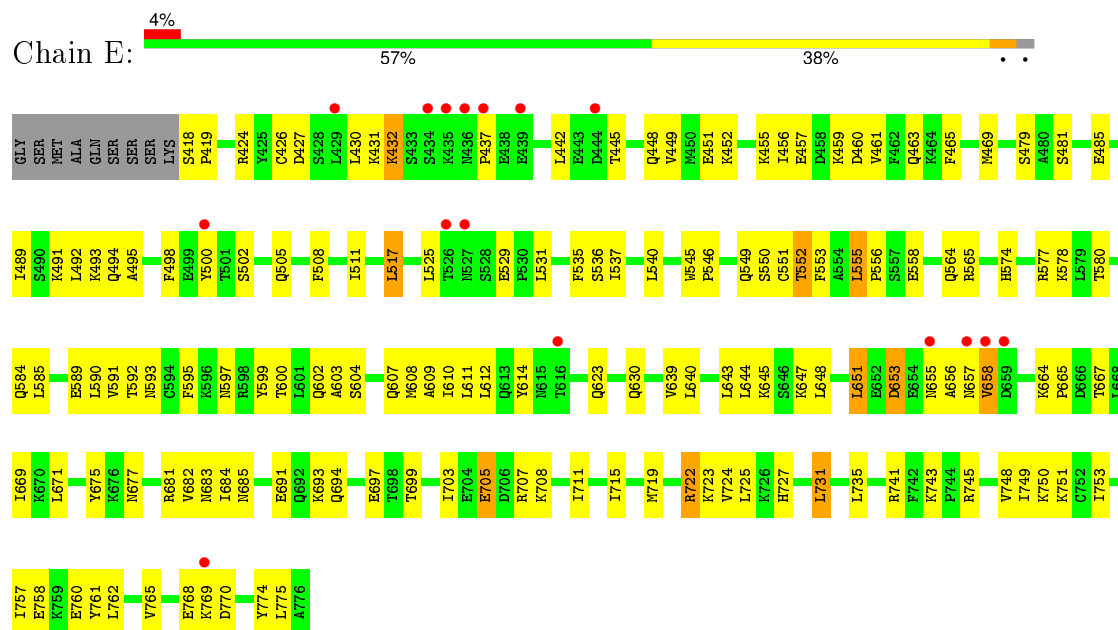
Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	EXPRESSION TAG	UNP P62877
B	4	SER	-	EXPRESSION TAG	UNP P62877
D	3	GLY	-	EXPRESSION TAG	UNP P62877
D	4	SER	-	EXPRESSION TAG	UNP P62877
F	3	GLY	-	EXPRESSION TAG	UNP P62877
F	4	SER	-	EXPRESSION TAG	UNP P62877
H	3	GLY	-	EXPRESSION TAG	UNP P62877
H	4	SER	-	EXPRESSION TAG	UNP P62877

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

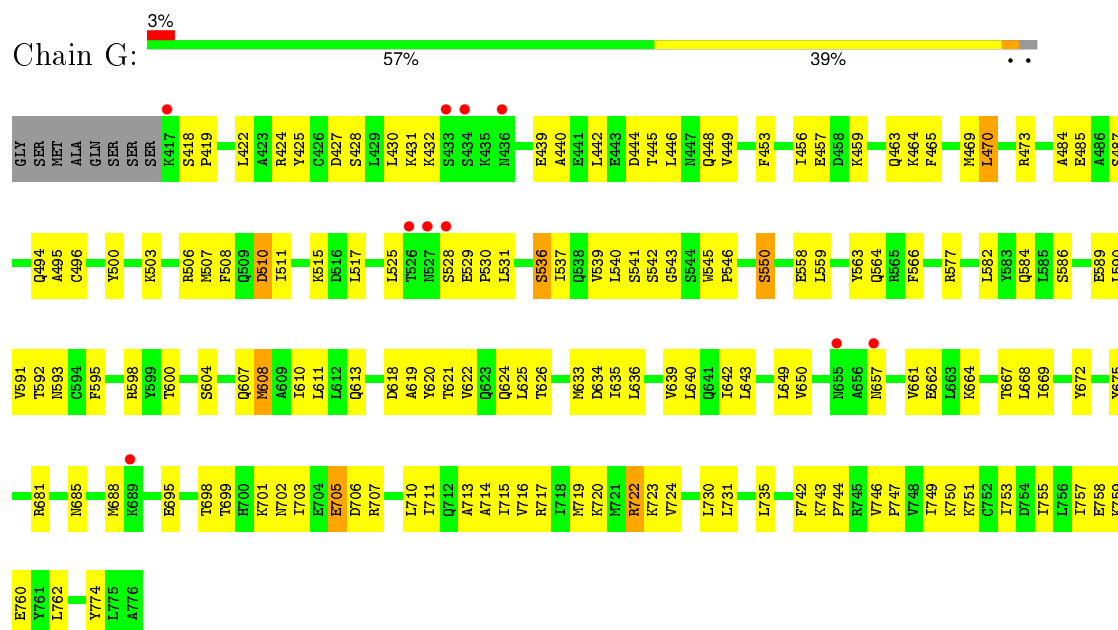
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	3	Total	Zn	0	0
			3	3		
3	B	3	Total	Zn	0	0
			3	3		
3	D	3	Total	Zn	0	0
			3	3		
3	F	3	Total	Zn	0	0
			3	3		



• Molecule 1: Cullin-1

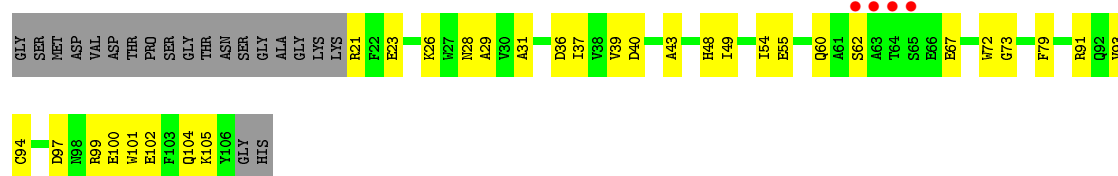


• Molecule 1: Cullin-1

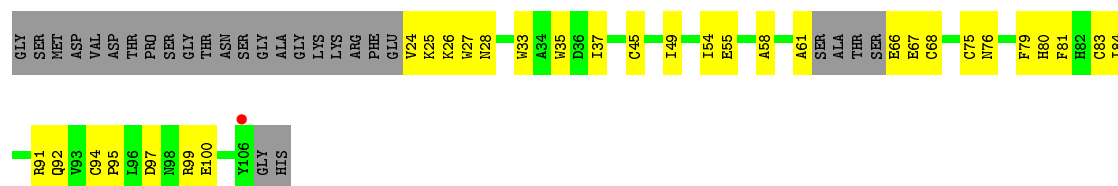


• Molecule 2: E3 ubiquitin-protein ligase RBX1

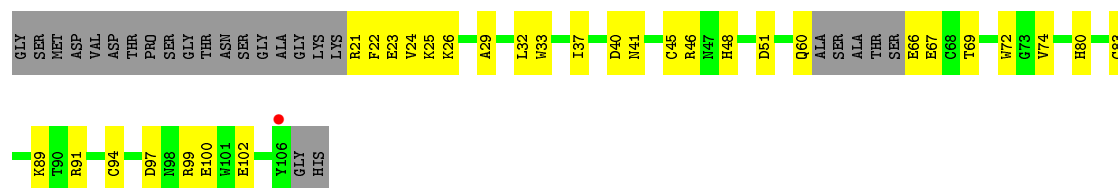




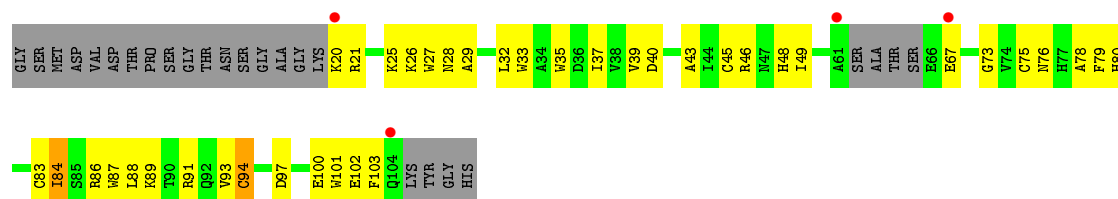
• Molecule 2: E3 ubiquitin-protein ligase RBX1



• Molecule 2: E3 ubiquitin-protein ligase RBX1



• Molecule 2: E3 ubiquitin-protein ligase RBX1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.47Å 119.80Å 231.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.21 29.95 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.21) 100.0 (29.95-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.238 , 0.282 0.229 , 0.278	Depositor DCC
R_{free} test set	2051 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	100.6	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 41053 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14055	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.37	0/2911	0.53	0/3910
1	C	0.37	0/2624	0.51	0/3509
1	E	0.36	0/2963	0.50	0/3983
1	G	0.39	0/2982	0.53	0/4006
2	B	0.44	0/734	0.56	0/998
2	D	0.54	1/677 (0.1%)	0.59	0/920
2	F	0.54	1/704 (0.1%)	0.59	0/955
2	H	0.48	0/690	0.55	0/937
All	All	0.40	2/14285 (0.0%)	0.53	0/19218

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	45	CYS	CB-SG	-5.71	1.72	1.81
2	F	45	CYS	CB-SG	-5.35	1.73	1.81

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	2870	0	2931	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2592	0	2644	138	0
1	E	2918	0	2966	134	0
1	G	2937	0	3001	127	0
2	B	713	0	663	36	0
2	D	658	0	612	30	0
2	F	684	0	635	37	0
2	H	671	0	620	37	0
3	B	3	0	0	0	0
3	D	3	0	0	0	0
3	F	3	0	0	0	0
3	H	3	0	0	0	0
All	All	14055	0	14072	579	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 21.

The worst 5 of 579 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:E:639:VAL:O	1:E:643:LEU:HD23	1.61	0.98
1:C:743:LYS:HE3	1:C:743:LYS:HA	1.42	0.97
1:A:427:ASP:HB2	1:A:469:MET:HG2	1.43	0.96
1:E:493:LYS:HZ3	1:E:505:GLN:NE2	1.67	0.92
1:E:493:LYS:HZ3	1:E:505:GLN:HE22	1.01	0.92

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	349/368 (95%)	314 (90%)	31 (9%)	4 (1%)	17 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	299/368 (81%)	264 (88%)	30 (10%)	5 (2%)	11	52
1	E	357/368 (97%)	320 (90%)	30 (8%)	7 (2%)	9	48
1	G	358/368 (97%)	318 (89%)	35 (10%)	5 (1%)	14	57
2	B	84/106 (79%)	75 (89%)	8 (10%)	1 (1%)	16	60
2	D	75/106 (71%)	70 (93%)	5 (7%)	0	100	100
2	F	77/106 (73%)	72 (94%)	5 (6%)	0	100	100
2	H	77/106 (73%)	68 (88%)	6 (8%)	3 (4%)	4	28
All	All	1676/1896 (88%)	1501 (90%)	150 (9%)	25 (2%)	13	55

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	658	VAL
1	A	723	LYS
1	E	723	LYS
1	G	550	SER
1	A	480	ALA

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	323/339 (95%)	317 (98%)	6 (2%)	65	88
1	C	292/339 (86%)	283 (97%)	9 (3%)	47	81
1	E	328/339 (97%)	321 (98%)	7 (2%)	61	87
1	G	332/339 (98%)	323 (97%)	9 (3%)	52	84
2	B	76/90 (84%)	76 (100%)	0	100	100
2	D	70/90 (78%)	69 (99%)	1 (1%)	74	91
2	F	73/90 (81%)	72 (99%)	1 (1%)	74	91
2	H	71/90 (79%)	69 (97%)	2 (3%)	51	83
All	All	1565/1716 (91%)	1530 (98%)	35 (2%)	60	87

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	68	CYS
1	E	651	LEU
1	G	722	ARG
1	E	517	LEU
1	E	555	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	505	GLN
1	E	607	GLN
1	G	593	ASN
2	D	48	HIS
1	G	564	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 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, 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	353/368 (95%)	0.06	8 (2%) 64 52	63, 124, 177, 210	0
1	C	317/368 (86%)	0.30	20 (6%) 23 14	74, 155, 196, 213	0
1	E	359/368 (97%)	0.23	16 (4%) 37 25	80, 138, 180, 211	0
1	G	360/368 (97%)	0.13	10 (2%) 56 44	58, 124, 183, 217	0
2	B	86/106 (81%)	0.33	4 (4%) 35 24	64, 83, 183, 212	0
2	D	79/106 (74%)	0.07	1 (1%) 79 69	49, 78, 165, 220	0
2	F	81/106 (76%)	0.09	1 (1%) 81 71	61, 84, 142, 167	0
2	H	81/106 (76%)	0.21	4 (4%) 33 22	74, 102, 147, 168	0
All	All	1716/1896 (90%)	0.18	64 (3%) 45 31	49, 128, 186, 220	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	63	ALA	6.5
1	G	433	SER	6.0
2	B	65	SER	5.4
1	G	434	SER	5.3
2	B	62	SER	5.2

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	B	202	1/1	0.99	0.23	0.27	74,74,74,74	0
3	ZN	H	203	1/1	0.97	0.22	0.16	98,98,98,98	0
3	ZN	B	206	1/1	0.99	0.20	-0.15	60,60,60,60	0
3	ZN	D	205	1/1	0.93	0.18	-0.21	68,68,68,68	0
3	ZN	D	201	1/1	0.99	0.22	-0.40	65,65,65,65	0
3	ZN	H	207	1/1	0.93	0.15	-0.76	82,82,82,82	0
3	ZN	F	204	1/1	0.99	0.21	-0.78	66,66,66,66	0
3	ZN	F	208	1/1	0.95	0.15	-0.83	71,71,71,71	0
3	ZN	F	212	1/1	0.98	0.15	-	74,74,74,74	0
3	ZN	H	211	1/1	0.94	0.14	-	106,106,106,106	0
3	ZN	B	210	1/1	0.95	0.16	-	88,88,88,88	0
3	ZN	D	209	1/1	0.96	0.20	-	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.