



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2024 – 01:38 AM EST

PDB ID : 3IHY
Title : Human PIK3C3 crystal structure
Authors : Siponen, M.I.; Tresaugues, L.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Kotzsch, A.; Kragh Nielsen, T.; Moche, M.; Nyman, T.; Persson, C.; Roos, A.K.; Sagemark, J.; Schueler, H.; Schutz, P.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Nordlund, P.; Structural Genomics Consortium (SGC)
Deposited on : 2009-07-31
Resolution : 2.80 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

<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 : 2.36
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)

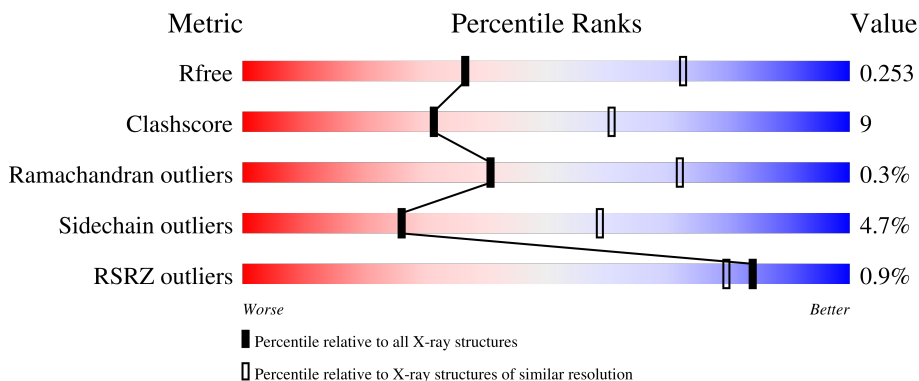
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

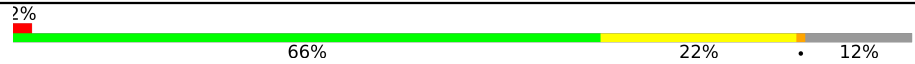

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	600	
1	B	600	
1	C	600	

Continued on next page...

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	D	600	 2% 66% 22% • 12%
1	E	600	 % 70% 16% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21670 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 Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	536	4343	2774	735	810	24	0	0	0
1	B	535	4339	2771	735	809	24	0	0	0
1	C	537	4344	2773	735	812	24	0	0	0
1	D	531	4303	2752	728	800	23	0	0	0
1	E	535	4340	2772	736	808	24	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8NEB9
A	-1	MET	-	expression tag	UNP Q8NEB9
B	-2	SER	-	expression tag	UNP Q8NEB9
B	-1	MET	-	expression tag	UNP Q8NEB9
C	-2	SER	-	expression tag	UNP Q8NEB9
C	-1	MET	-	expression tag	UNP Q8NEB9
D	280	SER	-	expression tag	UNP Q8NEB9
D	281	MET	-	expression tag	UNP Q8NEB9
E	-2	SER	-	expression tag	UNP Q8NEB9
E	-1	MET	-	expression tag	UNP Q8NEB9

- Molecule 2 is water.

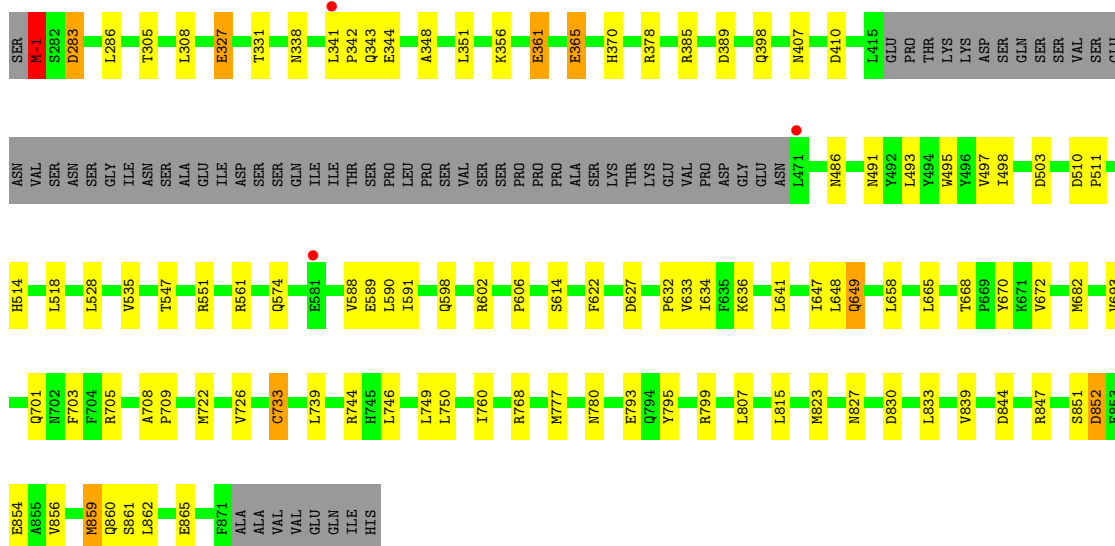
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	O	0	0
			1	1		

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.

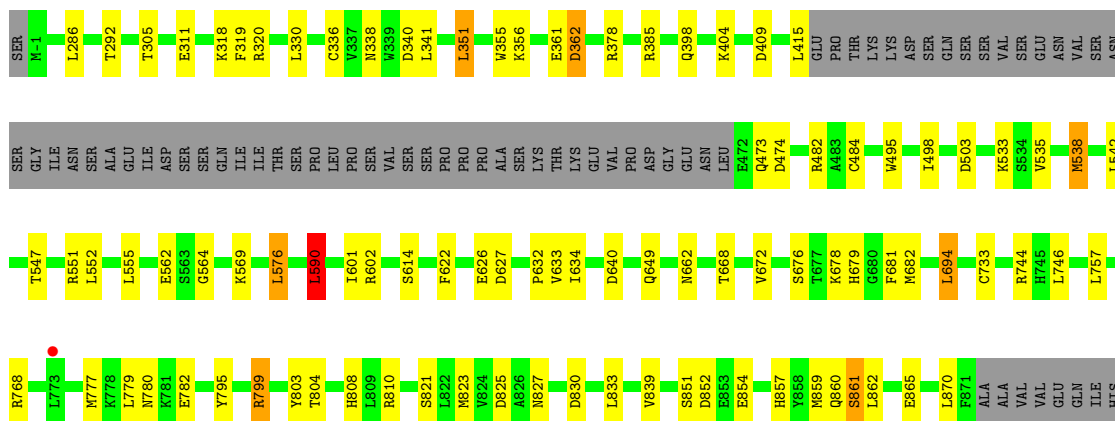
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain A: 



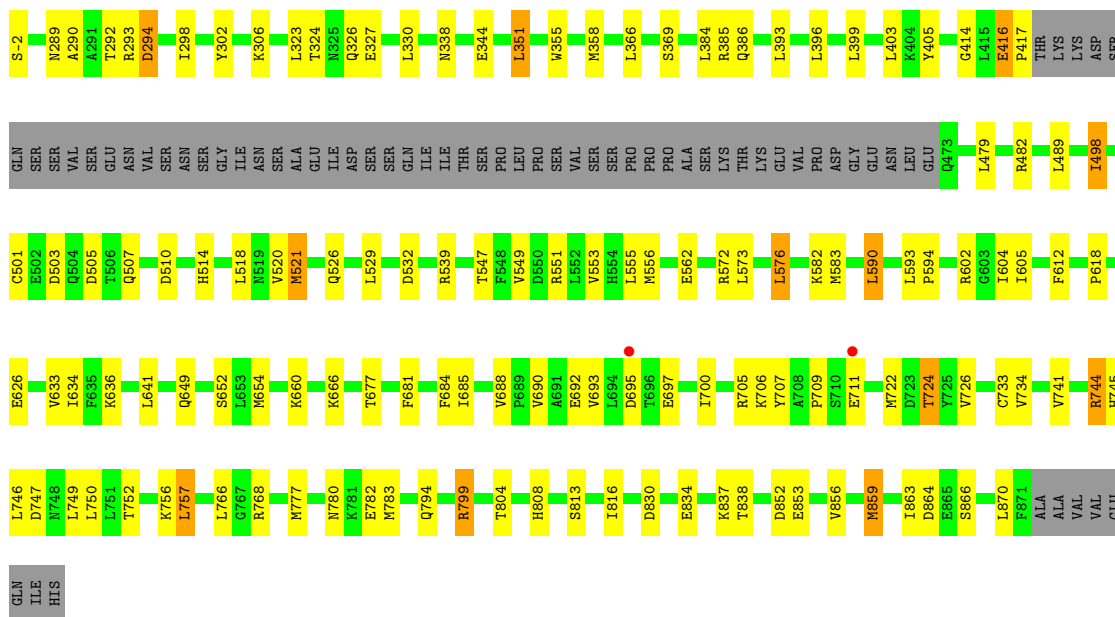
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain B: 



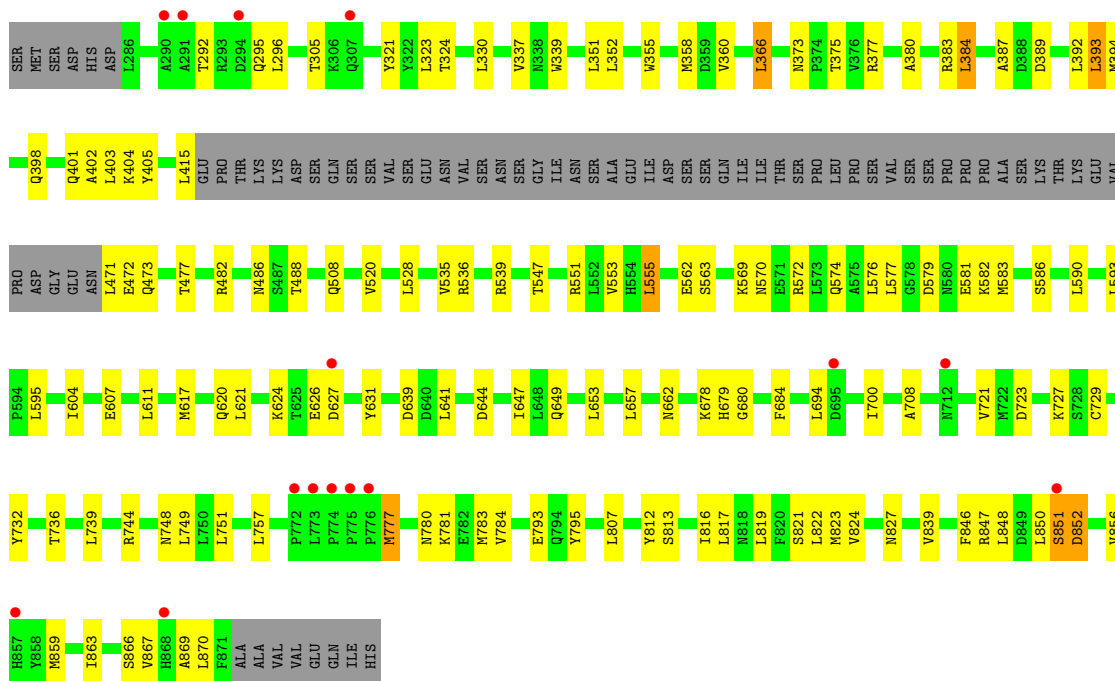
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain C: 



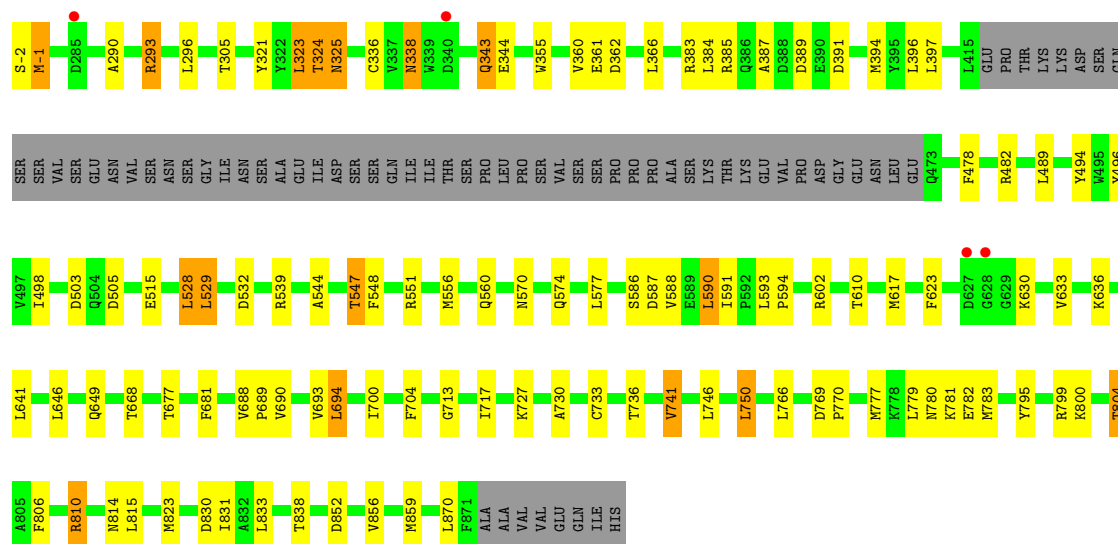
• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain D: 



• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain E: 



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.30Å 96.49Å 150.68Å 107.77° 91.75° 92.41°	Depositor
Resolution (Å)	19.84 – 2.80 19.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.84-2.80) 99.0 (19.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.79Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.255 0.190 , 0.253	Depositor DCC
R_{free} test set	4076 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.058 for -h,k,-k-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21670	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	0.72	2/4428 (0.0%)	0.75	1/5985 (0.0%)
1	B	0.71	1/4423 (0.0%)	0.80	5/5975 (0.1%)
1	C	0.65	1/4430 (0.0%)	0.73	2/5990 (0.0%)
1	D	0.59	0/4387	0.69	1/5930 (0.0%)
1	E	0.67	2/4425 (0.0%)	0.74	1/5978 (0.0%)
All	All	0.67	6/22093 (0.0%)	0.74	10/29858 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	MET	C-N	8.73	1.54	1.34
1	A	733	CYS	CB-SG	-5.95	1.72	1.81
1	E	336	CYS	CB-SG	-5.43	1.73	1.81
1	E	515	GLU	CG-CD	5.43	1.60	1.51
1	B	336	CYS	CB-SG	-5.21	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	482	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	482	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	415	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	-1	MET	C-N-CA	-5.41	108.16	121.70

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	4343	0	4380	74	0
1	B	4339	0	4376	53	0
1	C	4344	0	4370	93	0
1	D	4303	0	4348	83	0
1	E	4340	0	4390	89	0
2	B	1	0	0	0	0
All	All	21670	0	21864	390	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 9.

The worst 5 of 390 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:C:547:THR:HG22	1:C:551:ARG:NH1	1.67	1.08
1:D:749:LEU:HD21	1:D:783:MET:HE1	1.32	1.08
1:C:852:ASP:O	1:C:856:VAL:HG23	1.63	0.99
1:E:736:THR:HG22	1:E:741:VAL:HG11	1.47	0.96
1:C:734:VAL:HG22	1:C:859:MET:HE3	1.48	0.95

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	532/600 (89%)	502 (94%)	28 (5%)	2 (0%)	34 66
1	B	530/600 (88%)	510 (96%)	19 (4%)	1 (0%)	47 78
1	C	533/600 (89%)	506 (95%)	24 (4%)	3 (1%)	25 56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	527/600 (88%)	501 (95%)	24 (5%)	2 (0%)	34 66
1	E	531/600 (88%)	510 (96%)	21 (4%)	0	100 100
All	All	2653/3000 (88%)	2529 (95%)	116 (4%)	8 (0%)	41 72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	385	ARG
1	A	614	SER
1	D	852	ASP
1	C	711	GLU
1	B	590	LEU

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	483/543 (89%)	466 (96%)	17 (4%)	36 70
1	B	483/543 (89%)	454 (94%)	29 (6%)	19 48
1	C	483/543 (89%)	459 (95%)	24 (5%)	24 56
1	D	478/543 (88%)	459 (96%)	19 (4%)	31 65
1	E	484/543 (89%)	459 (95%)	25 (5%)	23 55
All	All	2411/2715 (89%)	2297 (95%)	114 (5%)	26 59

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	576	LEU
1	E	810	ARG
1	D	355	TRP
1	E	804	THR
1	E	366	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	-1:MET	C	282:SER	N	3.19

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	536/600 (89%)	-0.42	3 (0%) 89 86	19, 35, 54, 67	0
1	B	535/600 (89%)	-0.47	1 (0%) 95 94	18, 31, 47, 55	0
1	C	537/600 (89%)	-0.36	2 (0%) 92 91	20, 38, 54, 66	0
1	D	531/600 (88%)	-0.07	15 (2%) 53 43	35, 54, 70, 83	0
1	E	535/600 (89%)	-0.37	4 (0%) 87 84	21, 36, 50, 64	0
All	All	2674/3000 (89%)	-0.34	25 (0%) 84 80	18, 38, 63, 83	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	712	ASN	4.1
1	D	773	LEU	3.7
1	D	772	PRO	3.6
1	D	307	GLN	3.5
1	D	868	HIS	3.2

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.