



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2024 – 04:04 PM EST

PDB ID : 9C9I
Title : Structure of the TSC1:WIPI3 complex
Authors : D'Andrea, L.; Bayly-Jones, C.; Lupton, C.J.; Ellisdon, A.M.
Deposited on : 2024-06-14
Resolution : 3.18 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
Xtrriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

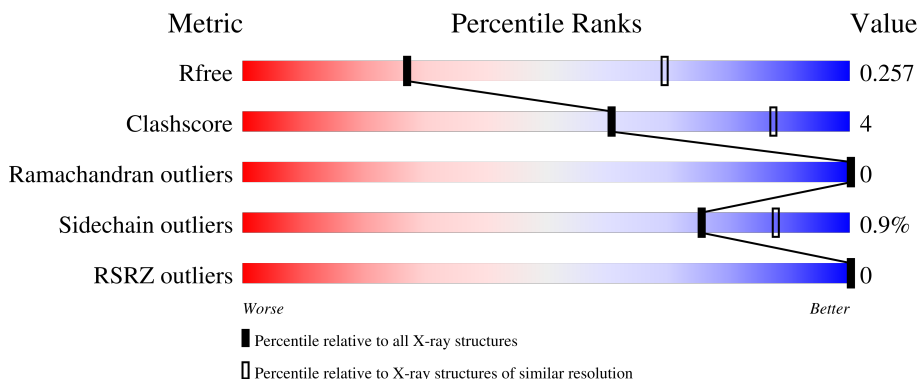
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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	316	85% 11% .
1	C	316	83% 13% .
1	E	316	84% 12% .
1	G	316	84% 11% .
2	B	34	59% 6% 35%

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Mol	Chain	Length	Quality of chain
2	D	34	 44% 56%
2	F	34	 56% 9% 35%
2	H	34	 47% 53%
2	X	34	 29% 68%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 10118 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 WD repeat domain phosphoinositide-interacting protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2372	1512	406	436	18	0	0	0
1	C	305	2372	1512	406	436	18	0	0	0
1	E	305	2372	1512	406	436	18	0	0	0
1	G	303	2354	1501	402	434	17	0	0	0

There are 124 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	MET	-	initiating methionine	UNP Q5MNZ6
A	6	HIS	-	expression tag	UNP Q5MNZ6
A	7	HIS	-	expression tag	UNP Q5MNZ6
A	8	HIS	-	expression tag	UNP Q5MNZ6
A	9	HIS	-	expression tag	UNP Q5MNZ6
A	10	HIS	-	expression tag	UNP Q5MNZ6
A	11	HIS	-	expression tag	UNP Q5MNZ6
A	?	-	PRO	deletion	UNP Q5MNZ6
A	?	-	LYS	deletion	UNP Q5MNZ6
A	?	-	TYR	deletion	UNP Q5MNZ6
A	?	-	PRO	deletion	UNP Q5MNZ6
A	?	-	PRO	deletion	UNP Q5MNZ6
A	?	-	ASN	deletion	UNP Q5MNZ6
A	?	-	ARG	deletion	UNP Q5MNZ6
A	?	-	ASN	deletion	UNP Q5MNZ6
A	?	-	LYS	deletion	UNP Q5MNZ6
A	?	-	GLN	deletion	UNP Q5MNZ6
A	?	-	SER	deletion	UNP Q5MNZ6
A	?	-	SER	deletion	UNP Q5MNZ6
A	?	-	LEU	deletion	UNP Q5MNZ6
A	?	-	ALA	deletion	UNP Q5MNZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q5MNZ6
A	?	-	ALA	deletion	UNP Q5MNZ6
A	?	-	SER	deletion	UNP Q5MNZ6
A	?	-	PHE	deletion	UNP Q5MNZ6
A	?	-	LEU	deletion	UNP Q5MNZ6
A	?	-	PRO	deletion	UNP Q5MNZ6
A	?	-	LYS	deletion	UNP Q5MNZ6
A	?	-	TYR	deletion	UNP Q5MNZ6
A	?	-	PHE	deletion	UNP Q5MNZ6
A	?	-	SER	deletion	UNP Q5MNZ6
C	5	MET	-	initiating methionine	UNP Q5MNZ6
C	6	HIS	-	expression tag	UNP Q5MNZ6
C	7	HIS	-	expression tag	UNP Q5MNZ6
C	8	HIS	-	expression tag	UNP Q5MNZ6
C	9	HIS	-	expression tag	UNP Q5MNZ6
C	10	HIS	-	expression tag	UNP Q5MNZ6
C	11	HIS	-	expression tag	UNP Q5MNZ6
C	?	-	PRO	deletion	UNP Q5MNZ6
C	?	-	LYS	deletion	UNP Q5MNZ6
C	?	-	TYR	deletion	UNP Q5MNZ6
C	?	-	PRO	deletion	UNP Q5MNZ6
C	?	-	PRO	deletion	UNP Q5MNZ6
C	?	-	ASN	deletion	UNP Q5MNZ6
C	?	-	ARG	deletion	UNP Q5MNZ6
C	?	-	ASN	deletion	UNP Q5MNZ6
C	?	-	LYS	deletion	UNP Q5MNZ6
C	?	-	GLN	deletion	UNP Q5MNZ6
C	?	-	SER	deletion	UNP Q5MNZ6
C	?	-	SER	deletion	UNP Q5MNZ6
C	?	-	LEU	deletion	UNP Q5MNZ6
C	?	-	ALA	deletion	UNP Q5MNZ6
C	?	-	SER	deletion	UNP Q5MNZ6
C	?	-	ALA	deletion	UNP Q5MNZ6
C	?	-	SER	deletion	UNP Q5MNZ6
C	?	-	PHE	deletion	UNP Q5MNZ6
C	?	-	LEU	deletion	UNP Q5MNZ6
C	?	-	PRO	deletion	UNP Q5MNZ6
C	?	-	LYS	deletion	UNP Q5MNZ6
C	?	-	TYR	deletion	UNP Q5MNZ6
C	?	-	PHE	deletion	UNP Q5MNZ6
C	?	-	SER	deletion	UNP Q5MNZ6
E	5	MET	-	initiating methionine	UNP Q5MNZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	6	HIS	-	expression tag	UNP Q5MNZ6
E	7	HIS	-	expression tag	UNP Q5MNZ6
E	8	HIS	-	expression tag	UNP Q5MNZ6
E	9	HIS	-	expression tag	UNP Q5MNZ6
E	10	HIS	-	expression tag	UNP Q5MNZ6
E	11	HIS	-	expression tag	UNP Q5MNZ6
E	?	-	PRO	deletion	UNP Q5MNZ6
E	?	-	LYS	deletion	UNP Q5MNZ6
E	?	-	TYR	deletion	UNP Q5MNZ6
E	?	-	PRO	deletion	UNP Q5MNZ6
E	?	-	PRO	deletion	UNP Q5MNZ6
E	?	-	ASN	deletion	UNP Q5MNZ6
E	?	-	ARG	deletion	UNP Q5MNZ6
E	?	-	ASN	deletion	UNP Q5MNZ6
E	?	-	LYS	deletion	UNP Q5MNZ6
E	?	-	GLN	deletion	UNP Q5MNZ6
E	?	-	SER	deletion	UNP Q5MNZ6
E	?	-	SER	deletion	UNP Q5MNZ6
E	?	-	LEU	deletion	UNP Q5MNZ6
E	?	-	ALA	deletion	UNP Q5MNZ6
E	?	-	SER	deletion	UNP Q5MNZ6
E	?	-	ALA	deletion	UNP Q5MNZ6
E	?	-	SER	deletion	UNP Q5MNZ6
E	?	-	PHE	deletion	UNP Q5MNZ6
E	?	-	LEU	deletion	UNP Q5MNZ6
E	?	-	PRO	deletion	UNP Q5MNZ6
E	?	-	LYS	deletion	UNP Q5MNZ6
E	?	-	TYR	deletion	UNP Q5MNZ6
E	?	-	PHE	deletion	UNP Q5MNZ6
E	?	-	SER	deletion	UNP Q5MNZ6
G	5	MET	-	initiating methionine	UNP Q5MNZ6
G	6	HIS	-	expression tag	UNP Q5MNZ6
G	7	HIS	-	expression tag	UNP Q5MNZ6
G	8	HIS	-	expression tag	UNP Q5MNZ6
G	9	HIS	-	expression tag	UNP Q5MNZ6
G	10	HIS	-	expression tag	UNP Q5MNZ6
G	11	HIS	-	expression tag	UNP Q5MNZ6
G	?	-	PRO	deletion	UNP Q5MNZ6
G	?	-	LYS	deletion	UNP Q5MNZ6
G	?	-	TYR	deletion	UNP Q5MNZ6
G	?	-	PRO	deletion	UNP Q5MNZ6
G	?	-	PRO	deletion	UNP Q5MNZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	ASN	deletion	UNP Q5MNZ6
G	?	-	ARG	deletion	UNP Q5MNZ6
G	?	-	ASN	deletion	UNP Q5MNZ6
G	?	-	LYS	deletion	UNP Q5MNZ6
G	?	-	GLN	deletion	UNP Q5MNZ6
G	?	-	SER	deletion	UNP Q5MNZ6
G	?	-	SER	deletion	UNP Q5MNZ6
G	?	-	LEU	deletion	UNP Q5MNZ6
G	?	-	ALA	deletion	UNP Q5MNZ6
G	?	-	SER	deletion	UNP Q5MNZ6
G	?	-	ALA	deletion	UNP Q5MNZ6
G	?	-	SER	deletion	UNP Q5MNZ6
G	?	-	PHE	deletion	UNP Q5MNZ6
G	?	-	LEU	deletion	UNP Q5MNZ6
G	?	-	PRO	deletion	UNP Q5MNZ6
G	?	-	LYS	deletion	UNP Q5MNZ6
G	?	-	TYR	deletion	UNP Q5MNZ6
G	?	-	PHE	deletion	UNP Q5MNZ6
G	?	-	SER	deletion	UNP Q5MNZ6

- Molecule 2 is a protein called Hamartin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	11	Total	C	N	O	0	0	0
			55	33	11	11			
2	B	22	Total	C	N	O	0	0	0
			176	114	31	31			
2	D	15	Total	C	N	O	0	0	0
			116	77	19	20			
2	F	22	Total	C	N	O	0	0	0
			176	114	31	31			
2	H	16	Total	C	N	O	0	0	0
			125	83	21	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	8	UNK	VAL	conflict	UNP Q92574
X	9	UNK	LEU	conflict	UNP Q92574
X	10	UNK	ASP	conflict	UNP Q92574
X	11	UNK	ARG	conflict	UNP Q92574
X	12	UNK	LEU	conflict	UNP Q92574

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Chain	Residue	Modelled	Actual	Comment	Reference
X	13	UNK	ILE	conflict	UNP Q92574
X	14	UNK	GLN	conflict	UNP Q92574
X	15	UNK	GLN	conflict	UNP Q92574
X	16	UNK	GLY	conflict	UNP Q92574
X	17	UNK	ALA	conflict	UNP Q92574
X	18	UNK	ASP	conflict	UNP Q92574
B	648	UNK	VAL	conflict	UNP Q92574
B	649	UNK	LEU	conflict	UNP Q92574
B	650	UNK	ASP	conflict	UNP Q92574
B	651	UNK	ARG	conflict	UNP Q92574
B	652	UNK	LEU	conflict	UNP Q92574
B	653	UNK	ILE	conflict	UNP Q92574
B	654	UNK	GLN	conflict	UNP Q92574
B	655	UNK	GLN	conflict	UNP Q92574
B	656	UNK	GLY	conflict	UNP Q92574
B	657	UNK	ALA	conflict	UNP Q92574
B	658	UNK	ASP	conflict	UNP Q92574
D	648	UNK	VAL	conflict	UNP Q92574
D	649	UNK	LEU	conflict	UNP Q92574
D	650	UNK	ASP	conflict	UNP Q92574
D	651	UNK	ARG	conflict	UNP Q92574
D	652	UNK	LEU	conflict	UNP Q92574
D	653	UNK	ILE	conflict	UNP Q92574
D	654	UNK	GLN	conflict	UNP Q92574
D	655	UNK	GLN	conflict	UNP Q92574
D	656	UNK	GLY	conflict	UNP Q92574
D	657	UNK	ALA	conflict	UNP Q92574
D	658	UNK	ASP	conflict	UNP Q92574
F	648	UNK	VAL	conflict	UNP Q92574
F	649	UNK	LEU	conflict	UNP Q92574
F	650	UNK	ASP	conflict	UNP Q92574
F	651	UNK	ARG	conflict	UNP Q92574
F	652	UNK	LEU	conflict	UNP Q92574
F	653	UNK	ILE	conflict	UNP Q92574
F	654	UNK	GLN	conflict	UNP Q92574
F	655	UNK	GLN	conflict	UNP Q92574
F	656	UNK	GLY	conflict	UNP Q92574
F	657	UNK	ALA	conflict	UNP Q92574
F	658	UNK	ASP	conflict	UNP Q92574
H	648	UNK	VAL	conflict	UNP Q92574
H	649	UNK	LEU	conflict	UNP Q92574
H	650	UNK	ASP	conflict	UNP Q92574

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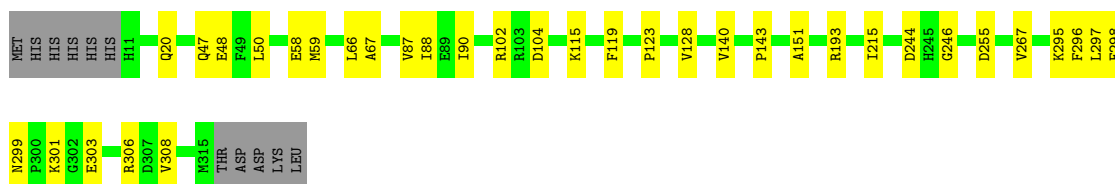
Chain	Residue	Modelled	Actual	Comment	Reference
H	651	UNK	ARG	conflict	UNP Q92574
H	652	UNK	LEU	conflict	UNP Q92574
H	653	UNK	ILE	conflict	UNP Q92574
H	654	UNK	GLN	conflict	UNP Q92574
H	655	UNK	GLN	conflict	UNP Q92574
H	656	UNK	GLY	conflict	UNP Q92574
H	657	UNK	ALA	conflict	UNP Q92574
H	658	UNK	ASP	conflict	UNP Q92574

3 Residue-property plots


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.

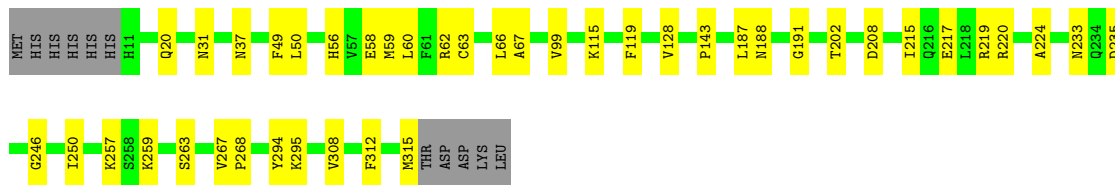
- Molecule 1: WD repeat domain phosphoinositide-interacting protein 3

Chain A: 




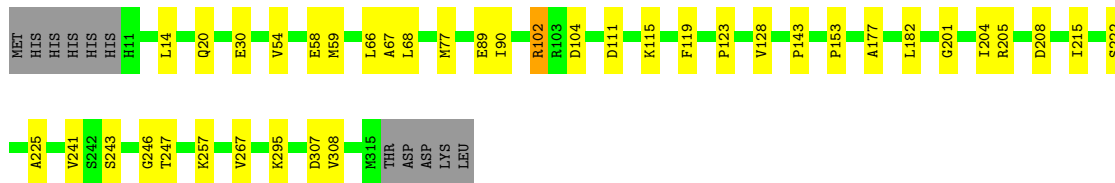
- Molecule 1: WD repeat domain phosphoinositide-interacting protein 3

Chain C: 




- Molecule 1: WD repeat domain phosphoinositide-interacting protein 3

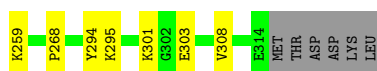
Chain E: 



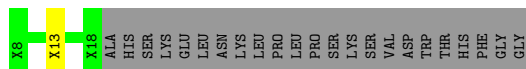
- Molecule 1: WD repeat domain phosphoinositide-interacting protein 3

Chain G: 

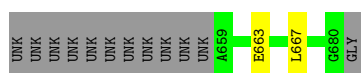




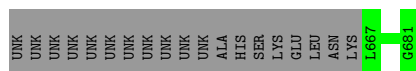
- Molecule 2: Hamartin



- Molecule 2: Hamartin



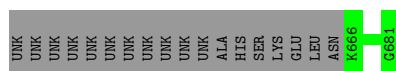
- Molecule 2: Hamartin



- Molecule 2: Hamartin



- Molecule 2: Hamartin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	94.24Å 94.24Å 199.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.12 – 3.18 47.12 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.5 (47.12-3.18) 99.3 (47.12-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.255 0.199 , 0.257	Depositor DCC
R_{free} test set	1495 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtrriage
Anisotropy	0.274	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10118	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0/2427	0.47	0/3283
1	C	0.25	0/2427	0.46	0/3283
1	E	0.25	0/2427	0.46	0/3283
1	G	0.25	0/2408	0.47	0/3258
2	B	0.23	0/182	0.45	0/246
2	D	0.23	0/121	0.41	0/165
2	F	0.21	0/182	0.42	0/246
2	H	0.23	0/130	0.43	0/176
All	All	0.25	0/10304	0.46	0/13940

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	2372	0	2345	19	0
1	C	2372	0	2345	23	0
1	E	2372	0	2345	22	0
1	G	2354	0	2329	18	0
2	B	176	0	173	1	0
2	D	116	0	110	0	0
2	F	176	0	173	2	0
2	H	125	0	123	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	55	0	14	1	0
All	All	10118	0	9957	83	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 4.

All (83) 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:A:297:LEU:HD12	1:A:306:ARG:HB2	1.68	0.76
1:C:58:GLU:HB3	1:C:67:ALA:HB3	1.73	0.70
1:E:20:GLN:HG2	1:E:143:PRO:HG3	1.72	0.69
1:G:58:GLU:HB3	1:G:67:ALA:HB3	1.75	0.69
1:C:20:GLN:HG2	1:C:143:PRO:HG3	1.73	0.68
1:A:115:LYS:HG2	1:A:128:VAL:HG22	1.78	0.66
1:G:20:GLN:HG2	1:G:143:PRO:HG3	1.78	0.66
1:C:208:ASP:HB2	1:C:215:ILE:HD11	1.78	0.64
1:C:295:LYS:HB3	1:C:308:VAL:HB	1.82	0.62
1:E:58:GLU:HB3	1:E:67:ALA:HB3	1.82	0.62
1:G:115:LYS:HG2	1:G:128:VAL:HG22	1.82	0.62
1:G:295:LYS:HB3	1:G:308:VAL:HB	1.83	0.60
1:E:115:LYS:HG2	1:E:128:VAL:HG12	1.82	0.60
1:E:59:MET:HG2	1:E:66:LEU:HD22	1.84	0.59
1:C:246:GLY:HA3	1:C:267:VAL:HG22	1.83	0.59
1:C:187:LEU:HD21	1:C:191:GLY:HA2	1.86	0.57
1:A:299:ASN:OD1	1:A:303:GLU:N	2.37	0.57
1:A:58:GLU:HB3	1:A:67:ALA:HB3	1.88	0.56
1:C:233:ASN:ND2	1:C:235:ASP:OD1	2.38	0.56
1:G:24:CYS:SG	1:G:62:ARG:NH1	2.79	0.55
1:C:115:LYS:HG2	1:C:128:VAL:HG22	1.88	0.55
1:E:204:ILE:HD13	1:E:241:VAL:HG21	1.87	0.55
1:G:29:MET:HG3	1:G:34:ARG:HH11	1.72	0.55
1:G:59:MET:HG2	1:G:66:LEU:HD22	1.88	0.54
1:C:59:MET:HG2	1:C:66:LEU:HD22	1.89	0.54
1:E:77:MET:HG2	1:E:89:GLU:HG2	1.90	0.53
1:A:59:MET:HG2	1:A:66:LEU:HD22	1.90	0.52
1:E:177:ALA:O	1:E:205:ARG:NH1	2.42	0.52
1:C:217:GLU:O	1:C:259:LYS:NZ	2.44	0.51
1:A:244:ASP:N	1:A:244:ASP:OD1	2.42	0.51
1:A:20:GLN:HG2	1:A:143:PRO:HG3	1.92	0.51
1:G:182:LEU:HD13	1:G:185:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASN:O	1:C:50:LEU:N	2.39	0.49
1:G:217:GLU:O	1:G:259:LYS:NZ	2.42	0.49
1:C:220:ARG:HG2	1:C:224:ALA:HB3	1.94	0.49
1:A:104:ASP:OD1	1:A:104:ASP:N	2.41	0.49
1:E:14:LEU:HD11	1:E:30:GLU:HG2	1.94	0.48
2:F:663:GLU:O	2:F:667:LEU:HG	2.13	0.48
1:G:162:LEU:HB2	1:G:173:VAL:HB	1.94	0.48
1:G:268:PRO:HD2	1:G:294:TYR:CE2	2.48	0.48
1:E:153:PRO:HB3	1:E:182:LEU:HD12	1.94	0.48
1:G:102:ARG:NH2	1:G:148:SER:OG	2.47	0.48
1:C:235:ASP:OD1	1:C:235:ASP:N	2.45	0.48
1:G:102:ARG:NH1	1:G:142:CYS:O	2.47	0.48
1:C:219:ARG:HG3	1:C:259:LYS:HE3	1.96	0.47
1:E:111:ASP:N	1:E:111:ASP:OD1	2.47	0.47
1:A:301:LYS:O	1:G:219:ARG:NH2	2.42	0.46
1:C:257:LYS:HG3	1:E:222:SER:HB3	1.97	0.46
1:A:255:ASP:N	1:A:255:ASP:OD1	2.49	0.46
2:B:663:GLU:O	2:B:667:LEU:HD13	2.15	0.45
1:A:296:PHE:HE1	1:A:298:PHE:HB3	1.82	0.45
1:E:307:ASP:O	2:X:13:UNK:N	2.50	0.45
1:G:87:VAL:HG23	1:G:88:ILE:HG13	1.99	0.45
1:C:37:ASN:OD1	1:C:62:ARG:NH2	2.49	0.45
1:E:243:SER:N	1:E:247:THR:O	2.47	0.45
1:G:201:GLY:O	1:G:220:ARG:NH1	2.50	0.45
1:A:48:GLU:C	1:A:50:LEU:H	2.20	0.44
1:G:301:LYS:HE3	1:G:303:GLU:OE1	2.16	0.44
1:E:102:ARG:NH1	1:E:104:ASP:OD1	2.50	0.44
1:E:295:LYS:HB3	1:E:308:VAL:HB	1.98	0.44
1:A:87:VAL:HG23	1:A:88:ILE:HG13	2.00	0.44
1:A:140:VAL:HG23	1:A:151:ALA:HB3	1.98	0.44
1:C:202:THR:OG1	1:C:219:ARG:NH2	2.49	0.44
1:E:20:GLN:NE2	1:E:59:MET:O	2.46	0.44
1:A:20:GLN:HB3	1:A:143:PRO:HG3	1.99	0.44
1:E:201:GLY:HA3	1:E:225:ALA:O	2.18	0.43
1:A:295:LYS:HB3	1:A:308:VAL:HB	1.99	0.43
1:E:54:VAL:HG11	1:E:68:LEU:HD22	2.01	0.43
1:E:90:ILE:HD11	1:E:123:PRO:HG2	2.01	0.43
2:F:659:ALA:O	2:F:663:GLU:HG3	2.19	0.43
1:C:250:ILE:HG12	1:C:263:SER:HB3	2.00	0.43
1:C:268:PRO:HD2	1:C:294:TYR:CE1	2.53	0.43
1:C:187:LEU:HD23	1:C:188:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:PHE:HA	1:C:315:MET:HG2	2.01	0.42
1:A:90:ILE:HD11	1:A:123:PRO:HG2	2.02	0.42
1:G:60:LEU:HB3	1:G:63:CYS:SG	2.60	0.42
1:E:208:ASP:HB2	1:E:215:ILE:HD11	2.02	0.41
1:E:246:GLY:HA3	1:E:267:VAL:HG22	2.03	0.41
1:C:60:LEU:HB3	1:C:63:CYS:SG	2.60	0.41
1:C:56:HIS:CD2	1:C:99:VAL:H	2.39	0.41
1:A:193:ARG:HG2	1:A:215:ILE:HD12	2.03	0.41
1:A:246:GLY:HA3	1:A:267:VAL:HG22	2.02	0.40
1:E:257:LYS:HE2	1:E:257:LYS:HB3	1.83	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	303/316 (96%)	276 (91%)	27 (9%)	0	100	100
1	C	303/316 (96%)	283 (93%)	20 (7%)	0	100	100
1	E	303/316 (96%)	282 (93%)	21 (7%)	0	100	100
1	G	301/316 (95%)	283 (94%)	18 (6%)	0	100	100
2	B	20/34 (59%)	19 (95%)	1 (5%)	0	100	100
2	D	13/34 (38%)	11 (85%)	2 (15%)	0	100	100
2	F	20/34 (59%)	19 (95%)	1 (5%)	0	100	100
2	H	14/34 (41%)	13 (93%)	1 (7%)	0	100	100
All	All	1277/1400 (91%)	1186 (93%)	91 (7%)	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	261/272 (96%)	258 (99%)	3 (1%)	70	84
1	C	261/272 (96%)	259 (99%)	2 (1%)	79	89
1	E	261/272 (96%)	259 (99%)	2 (1%)	79	89
1	G	259/272 (95%)	256 (99%)	3 (1%)	67	83
2	B	20/20 (100%)	20 (100%)	0	100	100
2	D	13/20 (65%)	13 (100%)	0	100	100
2	F	20/20 (100%)	20 (100%)	0	100	100
2	H	14/20 (70%)	14 (100%)	0	100	100
All	All	1109/1168 (95%)	1099 (99%)	10 (1%)	75	88

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	102	ARG
1	A	119	PHE
1	C	49	PHE
1	C	119	PHE
1	E	102	ARG
1	E	119	PHE
1	G	49	PHE
1	G	63	CYS
1	G	119	PHE

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 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 [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	305/316 (96%)	-1.42	0 100 100	72, 95, 142, 205	0
1	C	305/316 (96%)	-1.46	0 100 100	78, 107, 155, 194	0
1	E	305/316 (96%)	-1.42	0 100 100	69, 95, 138, 194	0
1	G	303/316 (95%)	-1.45	0 100 100	74, 108, 155, 181	0
2	B	22/34 (64%)	-1.33	0 100 100	91, 116, 175, 206	0
2	D	15/34 (44%)	-1.20	0 100 100	101, 113, 135, 137	0
2	F	22/34 (64%)	-1.37	0 100 100	103, 116, 156, 161	0
2	H	16/34 (47%)	-1.18	0 100 100	97, 115, 152, 156	0
2	X	0/34	-	-	-	-
All	All	1293/1434 (90%)	-1.43	0 100 100	69, 103, 154, 206	0

There are no RSRZ outliers to report.

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.