



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 10:37 PM EDT

PDB ID : 5HIU  
Title : Structure of the TSC2 N-terminus  
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Deposited on : 2016-01-12  
Resolution : 2.50 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](mailto: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>.

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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	:	2.37.1
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)	:	2.37.1

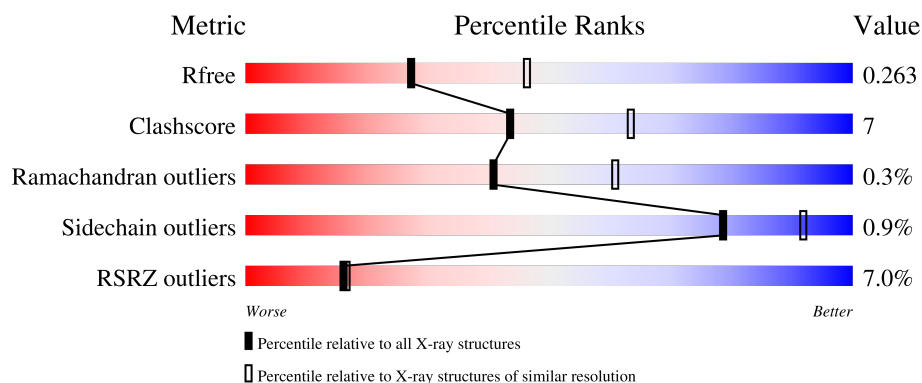
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	463	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>12%</div> </div> </div>
1	B	463	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>12%</div> </div> </div>
1	C	463	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>13%</div> </div> </div>
1	D	463	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>13%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12812 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 GTPase activator-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3222	2061	569	578	14			
1	B	407	Total	C	N	O	S	0	0	0
			3222	2059	569	580	14			
1	C	402	Total	C	N	O	S	0	0	0
			3188	2044	556	574	14			
1	D	401	Total	C	N	O	S	0	0	0
			3171	2035	549	573	14			

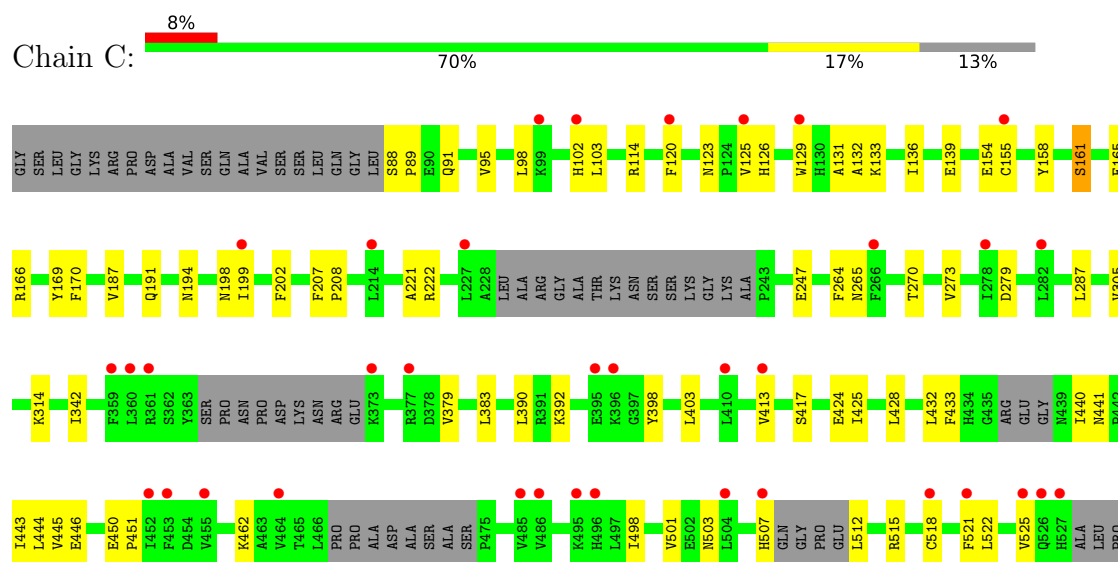
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	GLY	-	expression tag	UNP G0SFF5
A	69	SER	-	expression tag	UNP G0SFF5
B	68	GLY	-	expression tag	UNP G0SFF5
B	69	SER	-	expression tag	UNP G0SFF5
C	68	GLY	-	expression tag	UNP G0SFF5
C	69	SER	-	expression tag	UNP G0SFF5
D	68	GLY	-	expression tag	UNP G0SFF5
D	69	SER	-	expression tag	UNP G0SFF5

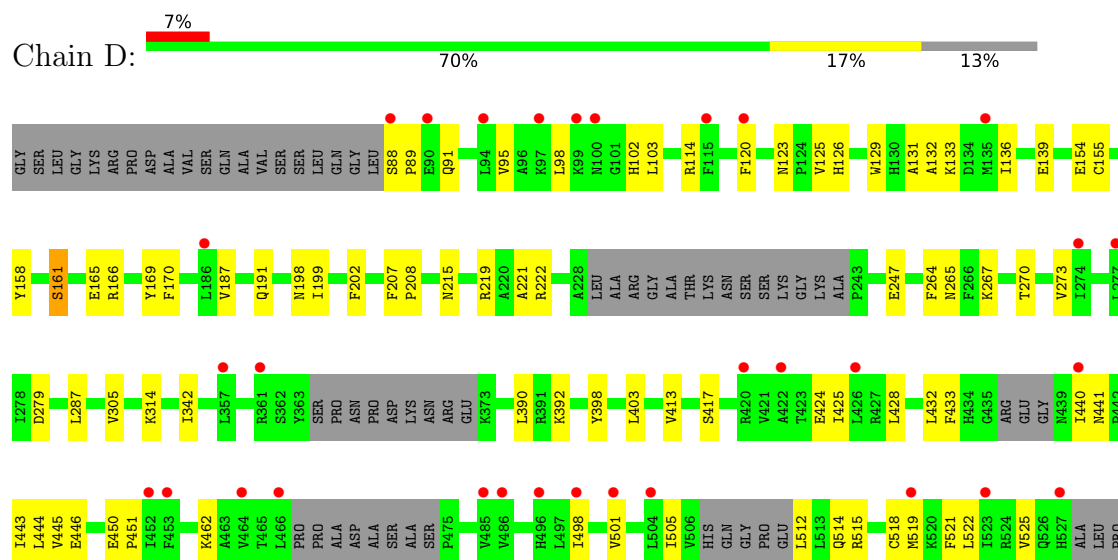
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	2	Total	O	0	0
			2	2		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		





• Molecule 1: GTPase activator-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.73Å 78.10Å 153.75Å 89.90° 89.85° 78.94°	Depositor
Resolution (Å)	41.90 – 2.50 41.94 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (41.90-2.50) 95.8 (41.94-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.224 , 0.263 0.233 , 0.263	Depositor DCC
$R_{free}$ test set	4219 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.459 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/3288	0.65	1/4458 (0.0%)
1	B	0.46	0/3288	0.65	1/4459 (0.0%)
1	C	0.41	0/3251	0.61	0/4408
1	D	0.40	0/3233	0.61	0/4386
All	All	0.44	0/13060	0.63	2/17711 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	186	LEU	CA-CB-CG	5.42	127.77	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	3222	0	3276	31	0
1	B	3222	0	3268	35	0
1	C	3188	0	3253	53	0
1	D	3171	0	3233	56	0
2	A	5	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1	0	0	0	0
All	All	12812	0	13030	174	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 7.

All (174) 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:433:PHE:HE1	1:C:444:LEU:HD22	1.42	0.85
1:C:433:PHE:CE1	1:C:444:LEU:HD22	2.17	0.80
1:D:433:PHE:CE1	1:D:444:LEU:HD22	2.18	0.79
1:A:291:GLU:OE2	1:A:331:SER:OG	2.02	0.78
1:D:433:PHE:HE1	1:D:444:LEU:HD22	1.47	0.78
1:B:403:LEU:HD11	1:B:452:ILE:HD11	1.67	0.77
1:A:403:LEU:HD11	1:A:452:ILE:HD11	1.66	0.76
1:A:498:ILE:HD11	1:A:525:VAL:HG11	1.69	0.73
1:B:498:ILE:HD11	1:B:525:VAL:HG11	1.70	0.72
1:D:287:LEU:HD12	1:D:287:LEU:O	1.90	0.72
1:C:287:LEU:HD12	1:C:287:LEU:O	1.89	0.72
1:B:291:GLU:OE2	1:B:331:SER:OG	2.07	0.71
1:D:133:LYS:O	1:D:136:ILE:HG12	1.93	0.69
1:A:182:PHE:CE2	1:A:186:LEU:HD23	2.30	0.67
1:C:133:LYS:O	1:C:136:ILE:HG12	1.94	0.67
1:B:182:PHE:CE2	1:B:186:LEU:HD23	2.29	0.67
1:C:512:LEU:O	1:C:515:ARG:HG3	1.96	0.65
1:C:433:PHE:CE1	1:C:444:LEU:CD2	2.80	0.64
1:D:512:LEU:O	1:D:515:ARG:HG3	1.96	0.64
1:D:433:PHE:CE1	1:D:444:LEU:CD2	2.80	0.64
1:C:433:PHE:HE1	1:C:444:LEU:CD2	2.10	0.64
1:D:445:VAL:HG23	1:D:446:GLU:HG2	1.81	0.63
1:B:287:LEU:O	1:B:287:LEU:HD12	1.98	0.62
1:D:433:PHE:HE1	1:D:444:LEU:CD2	2.12	0.62
1:D:417:SER:HB2	1:D:462:LYS:HE3	1.80	0.62
1:C:264:PHE:O	1:C:265:ASN:ND2	2.33	0.62
1:A:287:LEU:HD12	1:A:287:LEU:O	2.00	0.62
1:C:417:SER:HB2	1:C:462:LYS:HE3	1.80	0.62
1:C:445:VAL:HG23	1:C:446:GLU:HG2	1.82	0.62
1:A:387:GLN:OE1	1:A:427:ARG:HG2	2.00	0.60
1:C:126:HIS:CE1	1:C:165:GLU:HG2	2.36	0.59
1:B:407:VAL:HA	1:B:410:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ILE:HA	1:C:202:PHE:CE2	2.37	0.58
1:D:126:HIS:CE1	1:D:165:GLU:HG2	2.38	0.58
1:C:187:VAL:O	1:C:191:GLN:HG2	2.04	0.57
1:D:199:ILE:HA	1:D:202:PHE:CE2	2.40	0.57
1:D:264:PHE:O	1:D:265:ASN:ND2	2.39	0.56
1:B:361:ARG:HD3	1:B:405:LEU:HD12	1.87	0.56
1:B:387:GLN:OE1	1:B:427:ARG:HG2	2.06	0.56
1:C:440:ILE:HG23	1:C:444:LEU:HD11	1.88	0.55
1:C:170:PHE:CD2	1:C:202:PHE:CG	2.95	0.55
1:D:98:LEU:HD22	1:D:131:ALA:HB3	1.89	0.54
1:A:407:VAL:HA	1:A:410:LEU:HD12	1.88	0.54
1:D:187:VAL:O	1:D:191:GLN:HG2	2.07	0.54
1:C:501:VAL:HG12	1:C:522:LEU:HD11	1.90	0.54
1:D:170:PHE:CD2	1:D:202:PHE:CD2	2.96	0.54
1:C:428:LEU:C	1:C:428:LEU:HD23	2.28	0.54
1:D:170:PHE:CD2	1:D:202:PHE:CG	2.96	0.54
1:C:98:LEU:HD22	1:C:131:ALA:HB3	1.90	0.54
1:D:440:ILE:HG23	1:D:444:LEU:HD11	1.88	0.54
1:B:194:ASN:ND2	1:B:197:ARG:HD2	2.23	0.54
1:C:501:VAL:CG1	1:C:522:LEU:HD11	2.38	0.54
1:D:428:LEU:C	1:D:428:LEU:HD23	2.28	0.53
1:D:501:VAL:HG12	1:D:522:LEU:HD11	1.90	0.53
1:A:194:ASN:ND2	1:A:197:ARG:HD2	2.23	0.53
1:C:170:PHE:CD2	1:C:202:PHE:CD2	2.96	0.53
1:C:279:ASP:OD1	1:C:314:LYS:NZ	2.37	0.52
1:A:129:TRP:CE3	1:A:152:LEU:HD22	2.44	0.52
1:B:158:TYR:CZ	1:B:160:ASN:OD1	2.63	0.52
1:D:98:LEU:HD22	1:D:131:ALA:CB	2.39	0.52
1:D:501:VAL:CG1	1:D:522:LEU:HD11	2.39	0.52
1:D:279:ASP:OD1	1:D:314:LYS:NZ	2.40	0.52
1:D:305:VAL:HG23	1:D:342:ILE:HG21	1.92	0.51
1:B:129:TRP:CE3	1:B:152:LEU:HD22	2.46	0.51
1:C:98:LEU:HD22	1:C:131:ALA:CB	2.40	0.51
1:A:158:TYR:CZ	1:A:160:ASN:OD1	2.64	0.50
1:A:193:THR:HA	1:A:198:ASN:O	2.11	0.50
1:C:305:VAL:HG23	1:C:342:ILE:HG21	1.93	0.49
1:B:182:PHE:CE2	1:B:186:LEU:CD2	2.95	0.49
1:A:182:PHE:CE2	1:A:186:LEU:CD2	2.95	0.49
1:A:129:TRP:HZ2	1:A:172:THR:HB	1.78	0.48
1:C:392:LYS:HB3	1:C:398:TYR:CD1	2.49	0.48
1:C:166:ARG:NH2	1:C:198:ASN:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:ASN:O	1:C:507:HIS:N	2.40	0.48
1:D:170:PHE:CE2	1:D:202:PHE:CD2	3.02	0.48
1:B:358:ASP:O	1:B:362:SER:OG	2.31	0.48
1:D:125:VAL:HG21	1:D:155:CYS:O	2.14	0.47
1:C:498:ILE:HD11	1:C:525:VAL:HG11	1.97	0.47
1:D:518:CYS:O	1:D:522:LEU:HD12	2.15	0.47
1:D:392:LYS:HB3	1:D:398:TYR:CD1	2.49	0.47
1:A:406:LEU:HG	1:A:410:LEU:HD11	1.97	0.47
1:C:170:PHE:CE2	1:C:202:PHE:CD2	3.02	0.47
1:C:158:TYR:HD2	1:C:161:SER:HG	1.63	0.47
1:C:518:CYS:O	1:C:522:LEU:HD12	2.14	0.47
1:B:193:THR:HA	1:B:198:ASN:O	2.14	0.47
1:C:441:ASN:OD1	1:C:443:ILE:HG22	2.15	0.47
1:D:498:ILE:HD11	1:D:525:VAL:HG11	1.97	0.47
1:C:390:LEU:HD13	1:C:432:LEU:HD21	1.96	0.47
1:C:270:THR:OG1	1:C:273:VAL:HG23	2.15	0.47
1:A:358:ASP:O	1:A:362:SER:OG	2.33	0.46
1:B:129:TRP:HZ2	1:B:172:THR:HB	1.80	0.46
1:B:406:LEU:HG	1:B:410:LEU:HD11	1.97	0.46
1:A:375:THR:O	1:A:379:VAL:HG23	2.15	0.46
1:D:417:SER:HB2	1:D:462:LYS:CE	2.46	0.46
1:C:114:ARG:HG3	1:C:154:GLU:HG3	1.97	0.46
1:D:505:ILE:HD13	1:D:519:MET:HE2	1.98	0.46
1:D:132:ALA:O	1:D:133:LYS:C	2.54	0.46
1:D:158:TYR:HD2	1:D:161:SER:HG	1.63	0.46
1:D:390:LEU:HD13	1:D:432:LEU:HD21	1.98	0.46
1:A:441:ASN:OD1	1:A:443:ILE:HG22	2.15	0.46
1:C:125:VAL:HG21	1:C:155:CYS:O	2.14	0.46
1:D:114:ARG:HG3	1:D:154:GLU:HG3	1.98	0.46
1:A:489:ASN:O	1:A:492:LEU:N	2.43	0.46
1:C:120:PHE:HB3	1:C:123:ASN:CG	2.37	0.45
1:D:270:THR:OG1	1:D:273:VAL:HG23	2.16	0.45
1:B:445:VAL:HG23	1:B:446:GLU:HG2	1.98	0.45
1:C:91:GLN:O	1:C:95:VAL:HG23	2.17	0.45
1:D:120:PHE:HB3	1:D:123:ASN:CG	2.36	0.45
1:C:521:PHE:CE1	1:C:525:VAL:HG21	2.51	0.45
1:D:102:HIS:O	1:D:103:LEU:C	2.54	0.45
1:D:424:GLU:HA	1:D:424:GLU:OE1	2.16	0.45
1:D:521:PHE:CE1	1:D:525:VAL:HG21	2.51	0.45
1:C:433:PHE:CD1	1:C:444:LEU:HD21	2.53	0.44
1:C:102:HIS:O	1:C:103:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HG23	1:A:446:GLU:HG2	1.99	0.44
1:D:441:ASN:OD1	1:D:443:ILE:HG22	2.17	0.44
1:B:371:ARG:O	1:B:372:GLU:C	2.56	0.44
1:C:450:GLU:N	1:C:451:PRO:CD	2.81	0.44
1:D:222:ARG:HH11	1:D:287:LEU:HD13	1.83	0.44
1:B:207:PHE:CZ	1:B:261:VAL:HG12	2.53	0.43
1:C:132:ALA:O	1:C:133:LYS:C	2.55	0.43
1:D:91:GLN:O	1:D:95:VAL:HG23	2.17	0.43
1:A:426:LEU:HD21	1:A:459:CYS:HB2	2.00	0.43
1:D:450:GLU:N	1:D:451:PRO:CD	2.81	0.43
1:D:433:PHE:CD1	1:D:444:LEU:HD21	2.52	0.43
1:B:375:THR:O	1:B:379:VAL:HG23	2.18	0.43
1:A:371:ARG:O	1:A:372:GLU:C	2.57	0.43
1:B:426:LEU:HD21	1:B:459:CYS:HB2	2.00	0.43
1:C:222:ARG:HH11	1:C:287:LEU:HD13	1.84	0.43
1:D:514:GLN:O	1:D:515:ARG:C	2.57	0.43
1:B:433:PHE:HA	1:B:440:ILE:HD13	2.01	0.43
1:C:129:TRP:CZ2	1:C:169:TYR:HA	2.53	0.43
1:C:417:SER:HB2	1:C:462:LYS:CE	2.46	0.43
1:D:129:TRP:CZ2	1:D:169:TYR:HA	2.53	0.43
1:A:433:PHE:HA	1:A:440:ILE:HD13	2.00	0.42
1:A:510:PRO:HG2	1:B:146:GLN:HB3	2.01	0.42
1:D:390:LEU:O	1:D:441:ASN:ND2	2.49	0.42
1:A:304:LEU:HD23	1:A:304:LEU:HA	1.90	0.42
1:B:441:ASN:OD1	1:B:443:ILE:HG22	2.20	0.42
1:C:424:GLU:HA	1:C:424:GLU:OE1	2.19	0.42
1:D:207:PHE:N	1:D:208:PRO:CD	2.83	0.42
1:A:207:PHE:CZ	1:A:261:VAL:HG12	2.54	0.42
1:B:114:ARG:HD2	1:B:150:GLU:HB3	2.02	0.42
1:C:390:LEU:O	1:C:441:ASN:ND2	2.52	0.42
1:C:221:ALA:HA	1:C:247:GLU:HB3	2.02	0.42
1:B:129:TRP:CZ2	1:B:169:TYR:HA	2.55	0.42
1:B:390:LEU:O	1:B:441:ASN:ND2	2.47	0.42
1:B:489:ASN:O	1:B:492:LEU:N	2.46	0.42
1:B:508:GLN:CB	1:B:512:LEU:HB2	2.49	0.42
1:C:403:LEU:HB2	1:C:443:ILE:HG12	2.01	0.42
1:D:403:LEU:HB2	1:D:443:ILE:HG12	2.01	0.42
1:A:114:ARG:HD2	1:A:150:GLU:HB3	2.02	0.41
1:A:508:GLN:CB	1:A:512:LEU:HB2	2.50	0.41
1:D:215:ASN:O	1:D:219:ARG:HB2	2.20	0.41
1:B:407:VAL:HG22	1:B:452:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:GLU:O	1:A:451:PRO:C	2.59	0.41
1:B:102:HIS:O	1:B:105:GLU:N	2.51	0.41
1:A:407:VAL:HG22	1:A:452:ILE:HG12	2.02	0.41
1:A:457:ALA:O	1:A:460:ALA:HB3	2.21	0.41
1:B:450:GLU:O	1:B:451:PRO:C	2.59	0.41
1:C:88:SER:HB3	1:C:89:PRO:HD2	2.03	0.41
1:C:413:VAL:HG12	1:C:425:ILE:HD11	2.03	0.41
1:D:88:SER:HB3	1:D:89:PRO:HD2	2.03	0.41
1:D:166:ARG:NH2	1:D:198:ASN:O	2.54	0.41
1:C:207:PHE:N	1:C:208:PRO:CD	2.84	0.41
1:D:413:VAL:HG12	1:D:425:ILE:HD11	2.02	0.41
1:B:304:LEU:HD23	1:B:304:LEU:HA	1.90	0.40
1:D:221:ALA:HA	1:D:247:GLU:HB3	2.02	0.40
1:C:379:VAL:O	1:C:383:LEU:HD13	2.21	0.40
1:B:126:HIS:CE1	1:B:130:HIS:CE1	3.09	0.40
1:B:427:ARG:HA	1:B:493:GLN:OE1	2.21	0.40
1:A:357:LEU:O	1:A:360:LEU:N	2.52	0.40
1:D:267:LYS:N	1:D:267:LYS:HD3	2.36	0.40
1:D:433:PHE:CD1	1:D:444:LEU:CD2	3.04	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	397/463 (86%)	363 (91%)	32 (8%)	2 (0%)	29	48
1	B	397/463 (86%)	363 (91%)	32 (8%)	2 (0%)	29	48
1	C	390/463 (84%)	361 (93%)	28 (7%)	1 (0%)	41	61
1	D	389/463 (84%)	362 (93%)	27 (7%)	0	100	100
All	All	1573/1852 (85%)	1449 (92%)	119 (8%)	5 (0%)	41	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	SER
1	A	419	THR
1	B	416	SER
1	B	419	THR
1	C	194	ASN

### 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	356/402 (89%)	352 (99%)	4 (1%)	73	89
1	B	356/402 (89%)	351 (99%)	5 (1%)	67	86
1	C	355/402 (88%)	353 (99%)	2 (1%)	86	95
1	D	353/402 (88%)	351 (99%)	2 (1%)	86	95
All	All	1420/1608 (88%)	1407 (99%)	13 (1%)	78	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	SER
1	A	186	LEU
1	A	364	SER
1	A	373	LYS
1	B	167	SER
1	B	186	LEU
1	B	303	SER
1	B	364	SER
1	B	373	LYS
1	C	139	GLU
1	C	161	SER
1	D	139	GLU
1	D	161	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	HIS
1	A	194	ASN
1	A	526	GLN
1	B	178	HIS
1	B	194	ASN
1	C	102	HIS
1	C	137	HIS
1	C	265	ASN
1	C	326	HIS
1	C	347	HIS
1	D	102	HIS
1	D	137	HIS
1	D	326	HIS
1	D	347	HIS

### 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	407/463 (87%)	0.28	22 (5%)	25	27	44, 79, 127, 161	0
1	B	407/463 (87%)	0.32	24 (5%)	22	23	42, 78, 127, 161	0
1	C	402/463 (86%)	0.49	36 (8%)	9	9	61, 92, 128, 162	0
1	D	401/463 (86%)	0.43	31 (7%)	13	13	63, 92, 128, 173	0
All	All	1617/1852 (87%)	0.38	113 (6%)	16	16	42, 86, 128, 173	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	486	VAL	5.9
1	B	482	GLU	5.7
1	C	486	VAL	5.2
1	C	452	ILE	5.0
1	A	420	ARG	5.0
1	D	519	MET	5.0
1	D	464	VAL	4.6
1	D	527	HIS	4.6
1	D	504	LEU	4.5
1	B	229	LEU	4.3
1	D	453	PHE	4.2
1	C	227	LEU	4.2
1	C	507	HIS	4.2
1	A	419	THR	4.1
1	C	455	VAL	4.0
1	D	452	ILE	3.9
1	C	413	VAL	3.9
1	A	229	LEU	3.9
1	C	99	LYS	3.9
1	D	357	LEU	3.8
1	D	90	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	420	ARG	3.7
1	C	521	PHE	3.6
1	D	99	LYS	3.6
1	B	479	VAL	3.6
1	C	518	CYS	3.6
1	D	97	LYS	3.5
1	C	504	LEU	3.4
1	C	496	HIS	3.3
1	C	377	ARG	3.3
1	A	91	GLN	3.3
1	A	89	PRO	3.3
1	D	94	LEU	3.3
1	D	485	VAL	3.3
1	B	527	HIS	3.1
1	A	452	ILE	3.1
1	A	523	ILE	3.1
1	B	359	PHE	3.1
1	A	99	LYS	3.0
1	C	526	GLN	3.0
1	C	527	HIS	3.0
1	C	266	PHE	2.9
1	B	99	LYS	2.9
1	A	120	PHE	2.9
1	B	491	SER	2.9
1	C	120	PHE	2.9
1	C	464	VAL	2.9
1	C	525	VAL	2.9
1	D	88	SER	2.9
1	A	231	ARG	2.9
1	D	523	ILE	2.8
1	D	120	PHE	2.8
1	D	361	ARG	2.8
1	A	227	LEU	2.8
1	A	492	LEU	2.8
1	B	360	LEU	2.7
1	A	481	LYS	2.7
1	C	282	LEU	2.7
1	C	360	LEU	2.7
1	C	396	LYS	2.6
1	C	214	LEU	2.6
1	B	173	LEU	2.6
1	D	440	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	525	VAL	2.5
1	B	494	LEU	2.5
1	D	186	LEU	2.5
1	D	501	VAL	2.5
1	B	420	ARG	2.5
1	A	413	VAL	2.5
1	D	274	ILE	2.5
1	A	493	GLN	2.4
1	C	155	CYS	2.4
1	C	125	VAL	2.4
1	C	395	GLU	2.4
1	B	519	MET	2.4
1	A	122	LEU	2.4
1	C	453	PHE	2.4
1	A	527	HIS	2.4
1	B	378	ASP	2.3
1	C	373	LYS	2.3
1	D	115	PHE	2.3
1	C	278	ILE	2.3
1	C	495	LYS	2.3
1	C	129	TRP	2.3
1	D	100	ASN	2.3
1	C	359	PHE	2.2
1	B	395	GLU	2.2
1	C	485	VAL	2.2
1	C	102	HIS	2.2
1	D	422	ALA	2.2
1	A	395	GLU	2.2
1	C	410	LEU	2.2
1	B	525	VAL	2.2
1	D	426	LEU	2.2
1	B	526	GLN	2.2
1	C	361	ARG	2.2
1	B	481	LYS	2.1
1	D	466	LEU	2.1
1	A	462	LYS	2.1
1	A	519	MET	2.1
1	D	135	MET	2.1
1	B	413	VAL	2.1
1	B	120	PHE	2.1
1	B	361	ARG	2.1
1	B	498	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	498	ILE	2.1
1	B	97	LYS	2.1
1	A	186	LEU	2.1
1	D	277	LEU	2.1
1	B	457	ALA	2.0
1	C	199	ILE	2.0
1	B	227	LEU	2.0
1	D	496	HIS	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.