Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2016 – 06:40 PM EDT

PDB ID	:	5HIU
Title	:	Structure of the TSC2 N-terminus
Authors	:	Zech, R.; Kiontke, S.; Kummel, D.
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*
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:

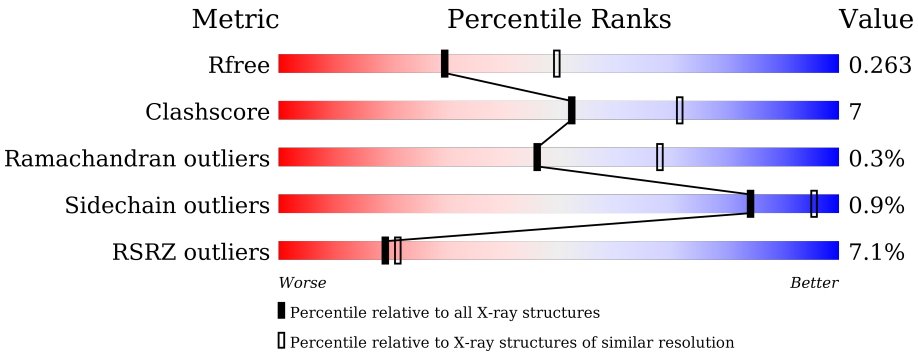
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 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 <=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	5% 75% 12% 12%
1	B	463	5% 74% 14% 12%
1	C	463	8% 70% 17% 13%
1	D	463	7% 70% 17% 13%

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.

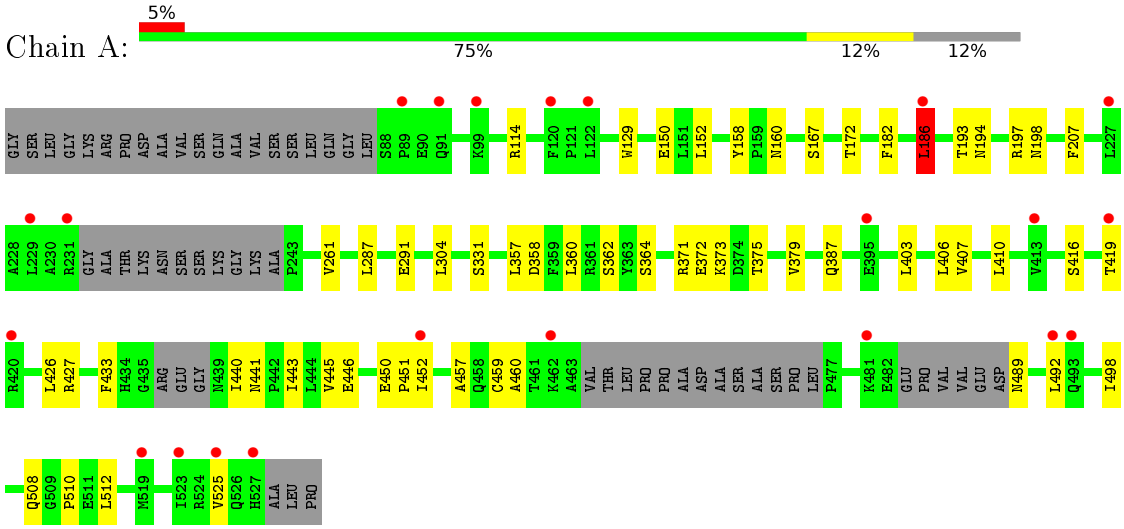
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	O	0	0
			5	5		
2	B	2	Total	O	0	0
			2	2		
2	C	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

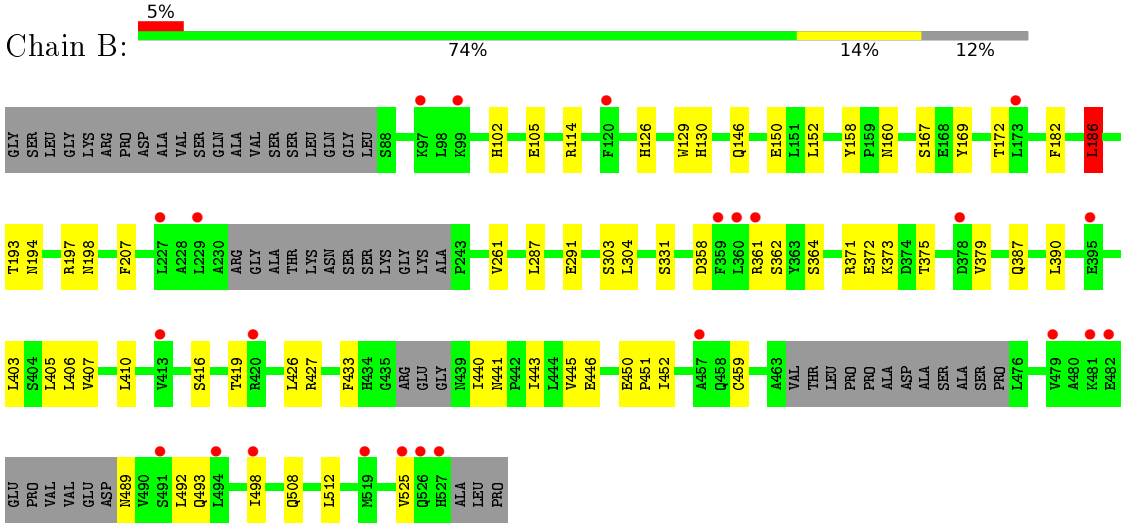
- Molecule 1: GTPase activator-like protein

Chain A:



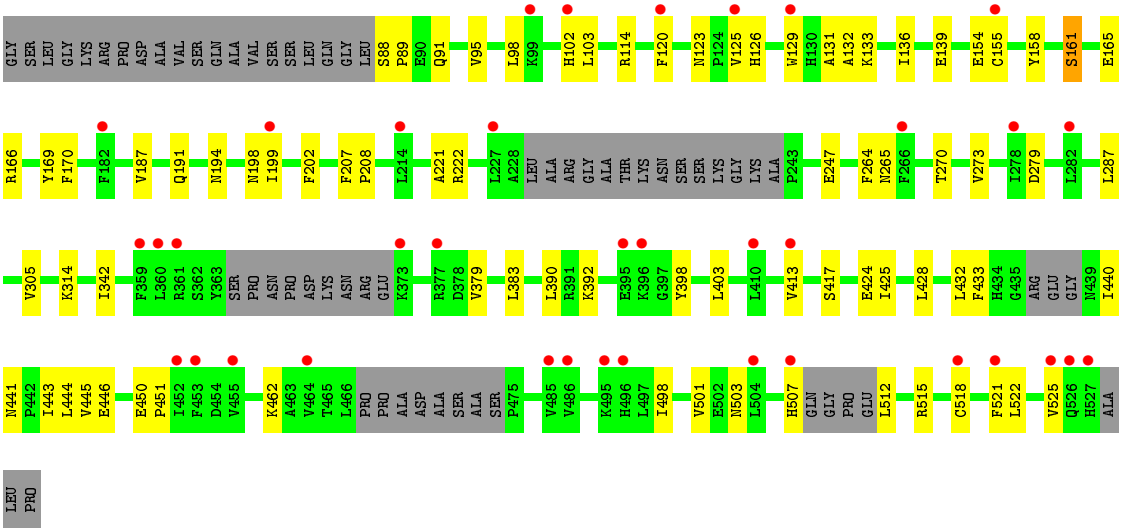
- Molecule 1: GTPase activator-like protein

Chain B:



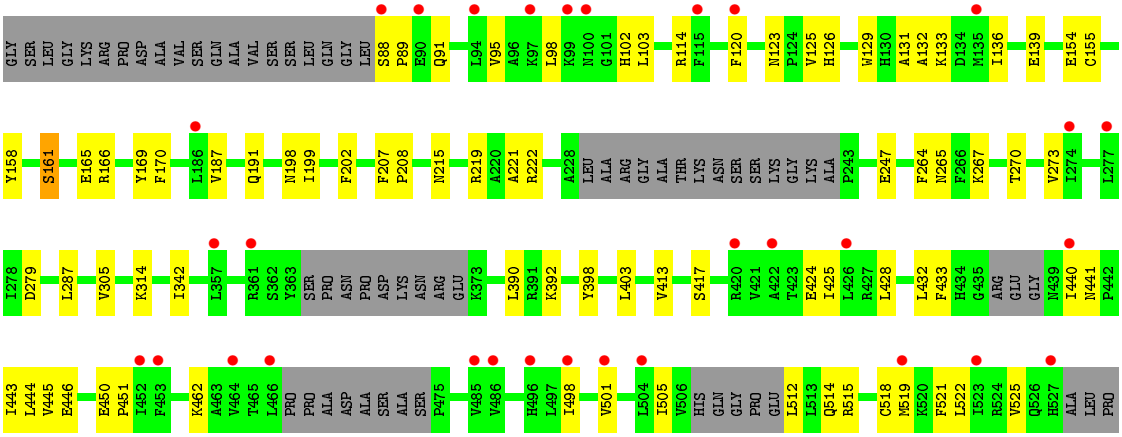
- Molecule 1: GTPase activator-like protein

Chain C:



- Molecule 1: GTPase activator-like protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	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) 95.9 (41.94-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	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	3326 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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

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:HD12	1:B:287:LEU:O	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:HD23	1:C:428:LEU:C	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:HD23	1:D:428:LEU:C	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:D:166:ARG:NH2	1:D:198:ASN:O	2.54	0.41
1:D:88:SER:HB3	1:D:89:PRO:HD2	2.03	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:413:VAL:HG12	1:C:425:ILE:HD11	2.03	0.41
1:C:88:SER:HB3	1:C:89:PRO:HD2	2.03	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:HD3	1:D:267:LYS:N	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 (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	397/463 (86%)	363 (91%)	32 (8%)	2 (0%)	34 55
1	B	397/463 (86%)	363 (91%)	32 (8%)	2 (0%)	34 55
1	C	390/463 (84%)	361 (93%)	28 (7%)	1 (0%)	46 68
1	D	389/463 (84%)	362 (93%)	27 (7%)	0	100 100
All	All	1573/1852 (85%)	1449 (92%)	119 (8%)	5 (0%)	46 68

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%)	80 94
1	B	356/402 (89%)	351 (99%)	5 (1%)	74 91
1	C	355/402 (88%)	353 (99%)	2 (1%)	90 97
1	D	353/402 (88%)	351 (99%)	2 (1%)	90 97
All	All	1420/1608 (88%)	1407 (99%)	13 (1%)	84 95

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

Some 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

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	407/463 (87%)	0.28	22 (5%)	29	33	44, 79, 127, 161	0
1	B	407/463 (87%)	0.31	24 (5%)	26	29	42, 78, 127, 161	0
1	C	402/463 (86%)	0.48	37 (9%)	11	12	61, 92, 128, 162	0
1	D	401/463 (86%)	0.43	31 (7%)	16	18	63, 92, 128, 173	0
All	All	1617/1852 (87%)	0.38	114 (7%)	19	21	42, 86, 128, 173	0

All (114) 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	A	420	ARG	5.1
1	C	452	ILE	5.1
1	D	519	MET	5.0
1	D	464	VAL	4.6
1	D	527	HIS	4.5
1	D	504	LEU	4.5
1	B	229	LEU	4.3
1	C	507	HIS	4.2
1	D	453	PHE	4.2
1	C	227	LEU	4.2
1	A	419	THR	4.1
1	C	455	VAL	4.0
1	D	452	ILE	3.9
1	A	229	LEU	3.9
1	C	99	LYS	3.9
1	C	413	VAL	3.8
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	3.6
1	D	99	LYS	3.6
1	C	521	PHE	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	A	91	GLN	3.3
1	C	377	ARG	3.3
1	A	89	PRO	3.2
1	D	94	LEU	3.2
1	D	485	VAL	3.2
1	B	527	HIS	3.1
1	A	452	ILE	3.1
1	A	523	ILE	3.1
1	B	359	PHE	3.0
1	C	527	HIS	3.0
1	A	99	LYS	3.0
1	C	526	GLN	3.0
1	C	266	PHE	2.9
1	B	99	LYS	2.9
1	A	120	PHE	2.9
1	C	464	VAL	2.9
1	B	491	SER	2.9
1	A	231	ARG	2.9
1	C	120	PHE	2.9
1	D	88	SER	2.8
1	C	525	VAL	2.8
1	D	523	ILE	2.8
1	D	361	ARG	2.8
1	A	227	LEU	2.8
1	D	120	PHE	2.7
1	A	492	LEU	2.7
1	A	481	LYS	2.7
1	B	360	LEU	2.7
1	C	282	LEU	2.7
1	C	396	LYS	2.7
1	C	360	LEU	2.6
1	C	214	LEU	2.6
1	A	525	VAL	2.5
1	B	173	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	440	ILE	2.5
1	B	494	LEU	2.5
1	D	501	VAL	2.5
1	D	186	LEU	2.5
1	B	420	ARG	2.5
1	C	155	CYS	2.4
1	A	413	VAL	2.4
1	C	125	VAL	2.4
1	D	274	ILE	2.4
1	C	395	GLU	2.4
1	A	493	GLN	2.4
1	B	519	MET	2.4
1	C	453	PHE	2.4
1	A	122	LEU	2.4
1	A	527	HIS	2.3
1	B	378	ASP	2.3
1	C	373	LYS	2.3
1	C	495	LYS	2.3
1	D	100	ASN	2.3
1	C	129	TRP	2.3
1	C	278	ILE	2.3
1	D	115	PHE	2.3
1	C	102	HIS	2.2
1	B	395	GLU	2.2
1	C	359	PHE	2.2
1	A	395	GLU	2.2
1	C	485	VAL	2.2
1	D	422	ALA	2.2
1	C	410	LEU	2.2
1	B	525	VAL	2.2
1	D	426	LEU	2.2
1	B	481	LYS	2.1
1	B	526	GLN	2.1
1	C	361	ARG	2.1
1	D	466	LEU	2.1
1	A	519	MET	2.1
1	D	135	MET	2.1
1	B	413	VAL	2.1
1	D	498	ILE	2.1
1	B	361	ARG	2.1
1	A	462	LYS	2.1
1	B	457	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	120	PHE	2.1
1	D	496	HIS	2.0
1	B	498	ILE	2.0
1	A	186	LEU	2.0
1	B	227	LEU	2.0
1	D	277	LEU	2.0
1	B	97	LYS	2.0
1	C	199	ILE	2.0
1	C	182	PHE	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 carbohydrates 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.