



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:53 am BST

PDB ID : 4M4E  
Title : TRAF domain of human TRAF4  
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Deposited on : 2013-08-07  
Resolution : 2.60 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.

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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 : 2.11  
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) : 2.11

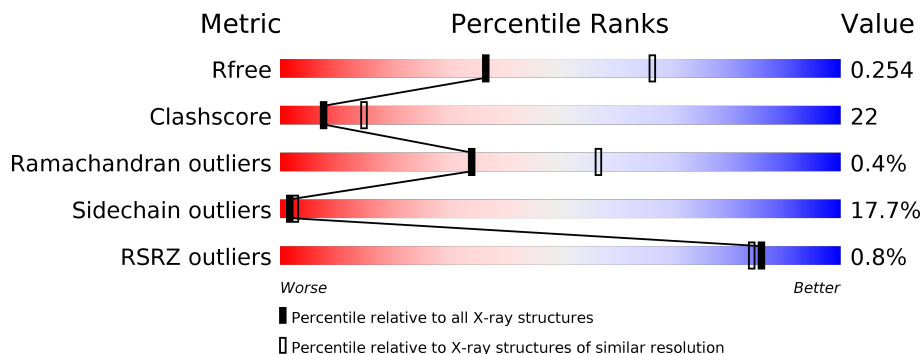
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	183	
1	B	183	
1	C	183	

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 4096 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 TNF receptor-associated factor 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1279	827	222	229	1	0	0	0
1	B	166	1338	861	233	243	1	0	0	0
1	C	170	1390	893	251	245	1	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	467	LEU	-	EXPRESSION TAG	UNP Q9BUZ4
A	468	GLU	-	EXPRESSION TAG	UNP Q9BUZ4
A	469	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
A	470	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
A	471	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
A	472	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
A	473	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
A	474	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	467	LEU	-	EXPRESSION TAG	UNP Q9BUZ4
B	468	GLU	-	EXPRESSION TAG	UNP Q9BUZ4
B	469	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	470	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	471	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	472	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	473	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
B	474	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
C	467	LEU	-	EXPRESSION TAG	UNP Q9BUZ4
C	468	GLU	-	EXPRESSION TAG	UNP Q9BUZ4
C	469	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
C	470	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
C	471	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
C	472	HIS	-	EXPRESSION TAG	UNP Q9BUZ4
C	473	HIS	-	EXPRESSION TAG	UNP Q9BUZ4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	474	HIS	-	EXPRESSION TAG	UNP Q9BUZ4

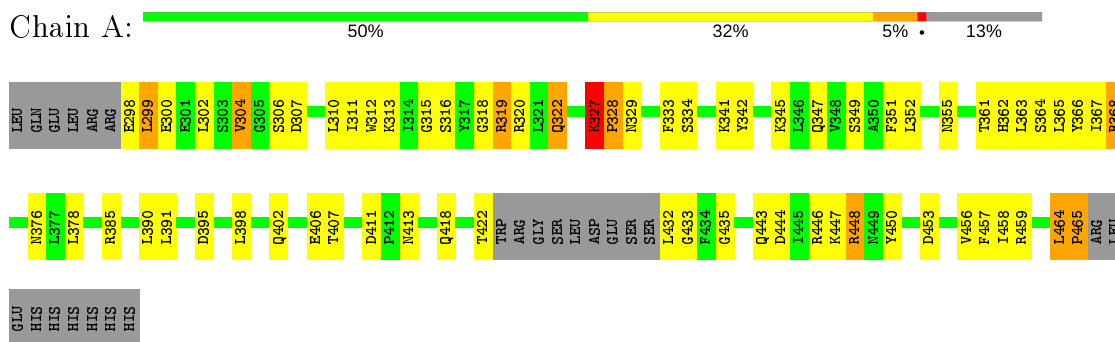
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	22	Total O 22 22	0	0
2	B	35	Total O 35 35	0	0
2	C	32	Total O 32 32	0	0

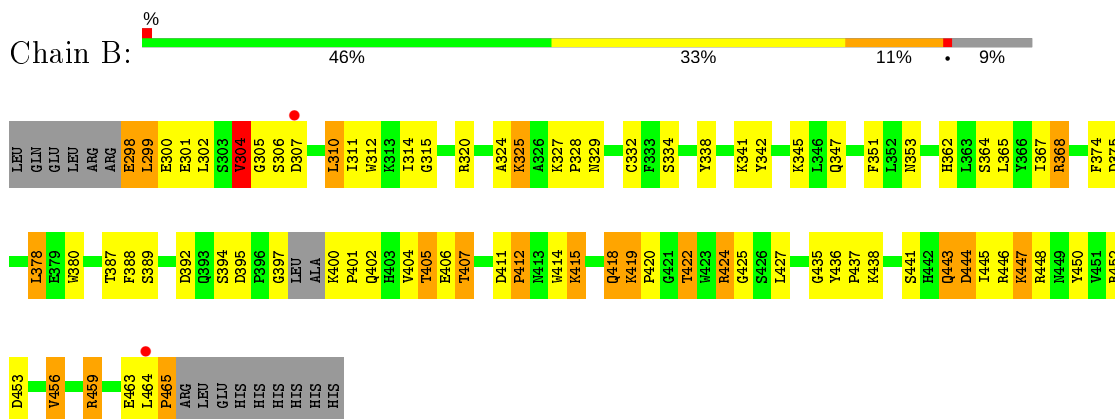
### 3 Residue-property plots [i](#)

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

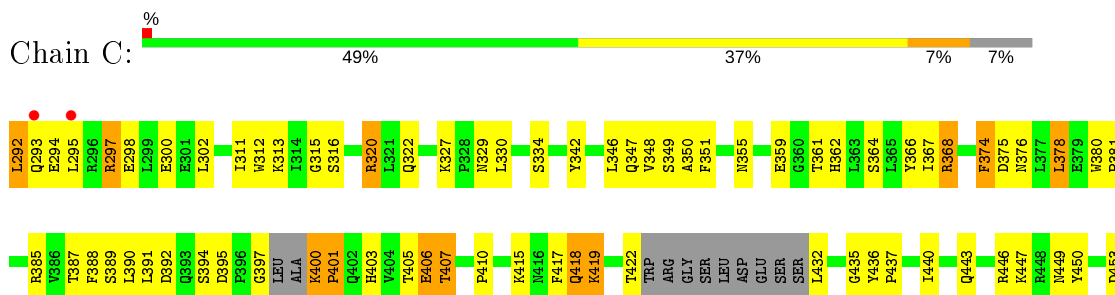
- Molecule 1: TNF receptor-associated factor 4



- Molecule 1: TNF receptor-associated factor 4



- Molecule 1: TNF receptor-associated factor 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.30Å 88.20Å 118.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.03 – 2.60 36.03 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.1 (36.03-2.60) 92.8 (36.03-2.59)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.25 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.200 , 0.277 0.218 , 0.254	Depositor DCC
$R_{free}$ test set	1846 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.8	Xtrriage
Anisotropy	0.727	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4096	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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	1.19	2/1317 (0.2%)	0.84	2/1784 (0.1%)
1	B	1.16	1/1378 (0.1%)	0.82	1/1866 (0.1%)
1	C	1.19	0/1431	0.81	0/1934
All	All	1.18	3/4126 (0.1%)	0.82	3/5584 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	465	PRO	N-CD	5.30	1.55	1.47
1	A	465	PRO	N-CD	5.25	1.55	1.47
1	A	328	PRO	N-CD	5.13	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	327	LYS	C-N-CD	5.80	140.59	128.40
1	B	464	LEU	C-N-CD	5.80	140.57	128.40
1	A	464	LEU	C-N-CD	5.42	139.78	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	304	VAL	Peptide



## 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	1279	0	1248	50	0
1	B	1338	0	1294	68	0
1	C	1390	0	1350	62	0
2	A	22	0	0	0	0
2	B	35	0	0	2	0
2	C	32	0	0	1	0
All	All	4096	0	3892	172	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 22.

All (172) 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:366:TYR:CD1	1:A:435:GLY:HA3	1.77	1.19
1:B:304:VAL:HG12	1:B:305:GLY:HA3	1.30	1.13
1:A:299:LEU:HA	1:A:302:LEU:HD23	1.30	1.13
1:A:368:ARG:HG2	1:A:368:ARG:HH11	1.18	1.05
1:C:366:TYR:CD1	1:C:435:GLY:HA3	1.96	1.00
1:B:301:GLU:OE2	1:B:338:TYR:OH	1.81	0.98
1:A:366:TYR:HD1	1:A:435:GLY:HA3	1.21	0.94
1:C:361:THR:HG1	1:C:362:HIS:HD1	1.01	0.90
1:B:300:GLU:OE2	1:B:345:LYS:NZ	2.06	0.88
1:B:299:LEU:HD13	1:B:299:LEU:H	1.38	0.87
1:C:376:ASN:OD1	1:C:419:LYS:NZ	2.09	0.86
1:B:304:VAL:CG1	1:B:305:GLY:HA3	2.07	0.84
1:C:400:LYS:HA	1:C:400:LYS:HE3	1.58	0.84
1:C:387:THR:HG23	1:C:407:THR:HG23	1.59	0.82
1:B:298:GLU:HB2	1:B:299:LEU:HD13	1.66	0.78
1:C:361:THR:HG1	1:C:362:HIS:CE1	2.01	0.78
1:B:387:THR:HG23	1:B:407:THR:HG22	1.68	0.75
1:B:415:LYS:HD2	1:B:418:GLN:NE2	2.03	0.74
1:A:453:ASP:OD1	1:C:376:ASN:ND2	2.20	0.74
1:B:425:GLY:O	2:B:535:HOH:O	2.06	0.74
1:B:299:LEU:HD13	1:B:299:LEU:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:LEU:O	1:C:403:HIS:HB3	1.90	0.72
1:C:366:TYR:HD1	1:C:435:GLY:HA3	1.49	0.71
1:A:299:LEU:HA	1:A:302:LEU:CD2	2.16	0.70
1:B:415:LYS:HD2	1:B:418:GLN:HE21	1.56	0.69
1:B:389:SER:OG	1:B:405:THR:HG22	1.95	0.67
1:C:361:THR:OG1	1:C:362:HIS:ND1	2.05	0.67
1:C:415:LYS:HD2	1:C:418:GLN:OE1	1.94	0.66
1:B:375:ASP:OD1	1:B:380:TRP:HZ2	1.77	0.66
1:A:367:ILE:O	1:A:433:GLY:HA3	1.96	0.66
1:B:389:SER:OG	1:B:405:THR:CG2	2.44	0.65
1:A:333:PHE:CD2	1:A:349:SER:OG	2.50	0.65
1:B:364:SER:OG	1:B:437:PRO:O	2.15	0.65
1:A:351:PHE:HB2	1:A:364:SER:HB2	1.78	0.65
1:A:361:THR:OG1	1:A:362:HIS:ND1	2.26	0.65
1:B:351:PHE:HB2	1:B:364:SER:HB2	1.79	0.65
1:C:415:LYS:CD	1:C:418:GLN:OE1	2.44	0.65
1:A:368:ARG:HG2	1:A:368:ARG:NH1	1.98	0.64
1:A:341:LYS:NZ	1:B:306:SER:HB2	2.11	0.64
1:C:292:LEU:HG	1:C:294:GLU:H	1.63	0.64
1:A:327:LYS:O	1:A:329:ASN:N	2.31	0.63
1:B:328:PRO:O	1:B:329:ASN:HB2	1.98	0.63
1:A:341:LYS:HG2	1:B:306:SER:HB2	1.81	0.62
1:C:327:LYS:HG2	1:C:327:LYS:O	1.99	0.62
1:B:400:LYS:HG3	1:B:401:PRO:HD2	1.83	0.61
1:A:411:ASP:OD1	1:A:413:ASN:HB2	2.01	0.60
1:C:389:SER:OG	1:C:405:THR:HG22	2.01	0.60
1:A:313:LYS:HE3	1:A:457:PHE:CZ	2.36	0.59
1:C:471:HIS:O	1:C:472:HIS:HB2	2.02	0.59
1:A:347:GLN:O	1:A:367:ILE:HG13	2.02	0.59
1:A:341:LYS:HG2	1:B:306:SER:CB	2.32	0.58
1:B:444:ASP:HA	1:B:447:LYS:HD2	1.85	0.58
1:C:351:PHE:CD1	1:C:355:ASN:HB2	2.39	0.58
1:A:316:SER:CB	1:A:319:ARG:NH1	2.67	0.58
1:A:352:LEU:HA	1:A:363:LEU:HD12	1.85	0.57
1:A:402:GLN:CD	1:A:448:ARG:NH1	2.58	0.57
1:C:315:GLY:O	1:C:316:SER:HB2	2.04	0.57
1:B:314:ILE:HB	1:B:456:VAL:HG23	1.87	0.56
1:A:300:GLU:OE1	1:A:345:LYS:NZ	2.38	0.56
1:B:306:SER:O	1:B:307:ASP:HB2	2.05	0.56
1:B:304:VAL:HG12	1:B:305:GLY:CA	2.20	0.56
1:A:333:PHE:CE2	1:A:349:SER:OG	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:SER:O	1:B:445:ILE:HG22	2.05	0.55
1:B:400:LYS:HG3	1:B:401:PRO:CD	2.36	0.55
1:C:364:SER:OG	1:C:437:PRO:O	2.23	0.55
1:C:450:TYR:O	1:C:456:VAL:HG12	2.07	0.55
1:A:368:ARG:CG	1:A:368:ARG:HH11	2.05	0.54
1:C:313:LYS:HD2	1:C:457:PHE:CE2	2.42	0.54
1:B:444:ASP:O	1:B:447:LYS:HB2	2.08	0.54
1:A:395:ASP:HB3	1:A:398:LEU:HD12	1.88	0.54
1:A:316:SER:O	1:A:320:ARG:HG3	2.08	0.53
1:A:402:GLN:NE2	1:A:448:ARG:NH1	2.56	0.53
1:A:318:GLY:O	1:A:322:GLN:HG3	2.09	0.53
1:B:422:THR:O	1:B:424:ARG:HG2	2.09	0.52
1:A:402:GLN:NE2	1:A:448:ARG:HH12	2.07	0.52
1:B:325:LYS:HG3	1:B:353:ASN:ND2	2.24	0.52
1:C:367:ILE:HB	1:C:388:PHE:HZ	1.75	0.52
1:A:316:SER:HB3	1:A:319:ARG:NH1	2.25	0.52
1:A:341:LYS:HZ2	1:B:306:SER:HB2	1.73	0.52
1:A:391:LEU:HD12	1:A:457:PHE:HB3	1.92	0.51
1:B:375:ASP:OD1	1:B:380:TRP:CZ2	2.61	0.51
1:C:297:ARG:HH21	1:C:298:GLU:HG2	1.74	0.51
1:C:312:TRP:CE3	1:C:334:SER:HB3	2.46	0.51
1:A:376:ASN:ND2	1:B:452:ARG:HG2	2.26	0.50
1:B:411:ASP:HB3	1:B:414:TRP:CD1	2.46	0.50
1:C:389:SER:HB2	1:C:459:ARG:HD2	1.94	0.50
1:B:324:ALA:O	1:B:327:LYS:O	2.29	0.50
1:C:419:LYS:O	1:C:422:THR:OG1	2.27	0.50
1:C:350:ALA:HA	1:C:364:SER:O	2.12	0.50
1:B:310:LEU:HD21	1:B:312:TRP:HB2	1.93	0.49
1:B:347:GLN:OE1	1:B:368:ARG:NH1	2.45	0.49
1:B:380:TRP:CD1	1:B:419:LYS:HG3	2.47	0.49
1:C:313:LYS:HD2	1:C:457:PHE:CZ	2.47	0.49
1:B:392:ASP:HB2	1:B:450:TYR:CE1	2.47	0.49
1:C:391:LEU:HD12	1:C:457:PHE:HB3	1.94	0.49
1:A:313:LYS:HE3	1:A:457:PHE:HZ	1.78	0.49
1:C:395:ASP:C	1:C:397:GLY:H	2.16	0.49
1:C:400:LYS:CA	1:C:400:LYS:HE3	2.24	0.49
1:C:470:HIS:ND1	1:C:471:HIS:N	2.60	0.49
1:B:375:ASP:HA	1:B:378:LEU:HD22	1.95	0.49
1:A:366:TYR:CE1	1:A:435:GLY:HA3	2.42	0.48
1:C:387:THR:OG1	1:C:407:THR:HG22	2.12	0.48
1:B:299:LEU:N	1:B:299:LEU:CD1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:ASP:O	1:B:397:GLY:N	2.46	0.48
1:B:362:HIS:CD2	1:B:438:LYS:HB3	2.49	0.48
1:C:400:LYS:HA	1:C:400:LYS:CE	2.38	0.47
1:B:365:LEU:O	1:B:435:GLY:HA3	2.14	0.47
1:C:334:SER:O	1:C:347:GLN:NE2	2.31	0.47
1:B:387:THR:CG2	1:B:407:THR:HG22	2.43	0.47
1:A:444:ASP:OD1	1:A:447:LYS:HE3	2.15	0.46
1:A:327:LYS:HB2	1:A:327:LYS:HE2	1.65	0.46
1:B:459:ARG:HD2	2:B:509:HOH:O	2.15	0.46
1:B:367:ILE:HB	1:B:388:PHE:HZ	1.81	0.46
1:A:341:LYS:HG3	1:A:342:TYR:CE1	2.51	0.46
1:C:320:ARG:HG2	1:C:320:ARG:HH11	1.80	0.46
1:C:391:LEU:HB2	1:C:457:PHE:HB2	1.98	0.46
1:A:302:LEU:O	1:A:304:VAL:HG23	2.16	0.45
1:B:342:TYR:HA	1:B:374:PHE:CD2	2.52	0.45
1:B:402:GLN:HG3	1:B:448:ARG:NH2	2.30	0.45
1:C:380:TRP:HA	1:C:381:PRO:C	2.36	0.45
1:B:310:LEU:HG	1:B:311:ILE:N	2.31	0.45
1:A:363:LEU:HG	1:A:364:SER:N	2.32	0.45
1:B:389:SER:HA	1:B:404:VAL:O	2.17	0.45
1:C:410:PRO:HB3	1:C:417:PHE:CE1	2.51	0.45
1:C:387:THR:HG23	1:C:407:THR:CG2	2.39	0.44
1:A:341:LYS:HZ3	1:B:306:SER:HB2	1.79	0.44
1:B:402:GLN:HG3	1:B:448:ARG:CZ	2.48	0.44
1:B:422:THR:O	1:B:424:ARG:CG	2.66	0.44
1:B:453:ASP:N	1:B:453:ASP:OD1	2.51	0.44
1:C:375:ASP:HA	1:C:378:LEU:HD22	1.99	0.44
1:C:346:LEU:HA	1:C:368:ARG:O	2.18	0.43
1:C:389:SER:OG	1:C:405:THR:CG2	2.65	0.43
1:B:415:LYS:HA	1:B:418:GLN:HE21	1.82	0.43
1:B:415:LYS:HA	1:B:418:GLN:HG3	2.01	0.43
1:C:472:HIS:HD2	2:C:521:HOH:O	2.02	0.43
1:C:342:TYR:HA	1:C:374:PHE:CD2	2.53	0.43
1:B:406:GLU:HA	1:B:406:GLU:OE2	2.18	0.43
1:C:348:VAL:HG12	1:C:349:SER:N	2.32	0.43
1:C:400:LYS:HA	1:C:401:PRO:HD3	1.85	0.43
1:C:436:TYR:HA	1:C:437:PRO:HD3	1.91	0.43
1:C:470:HIS:CG	1:C:471:HIS:N	2.87	0.43
1:C:470:HIS:CG	1:C:471:HIS:H	2.36	0.43
1:C:394:SER:HB2	1:C:401:PRO:HB3	2.01	0.43
1:C:415:LYS:HD3	1:C:418:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HG	1:A:311:ILE:N	2.33	0.42
1:A:315:GLY:O	1:A:316:SER:HB2	2.18	0.42
1:A:312:TRP:CE3	1:A:334:SER:HB3	2.54	0.42
1:A:390:LEU:HD21	1:A:450:TYR:HB3	2.01	0.42
1:C:330:LEU:HA	1:C:330:LEU:HD12	1.81	0.42
1:C:298:GLU:O	1:C:302:LEU:HD23	2.20	0.42
1:B:315:GLY:O	1:B:320:ARG:HD2	2.20	0.42
1:B:342:TYR:CE2	1:C:311:ILE:HB	2.55	0.42
1:A:365:LEU:HD21	1:A:458:ILE:HD12	2.01	0.42
1:B:419:LYS:HA	1:B:420:PRO:HD3	1.92	0.41
1:B:436:TYR:HA	1:B:437:PRO:HD2	1.82	0.41
1:B:443:GLN:CD	1:B:443:GLN:H	2.22	0.41
1:C:415:LYS:HD2	1:C:418:GLN:HG3	2.00	0.41
1:C:471:HIS:C	1:C:471:HIS:ND1	2.73	0.41
1:C:297:ARG:O	1:C:300:GLU:HB3	2.20	0.41
1:C:389:SER:HB2	1:C:459:ARG:HB3	2.02	0.41
1:A:341:LYS:O	1:A:341:LYS:HD2	2.20	0.41
1:B:368:ARG:H	1:B:368:ARG:HG3	1.77	0.41
1:B:441:SER:OG	1:B:444:ASP:OD1	2.38	0.41
1:B:392:ASP:HB2	1:B:450:TYR:HE1	1.84	0.41
1:A:306:SER:O	1:A:307:ASP:HB2	2.21	0.41
1:B:411:ASP:HA	1:B:412:PRO:HD2	1.90	0.41
1:A:368:ARG:CG	1:A:368:ARG:NH1	2.72	0.41
1:B:415:LYS:O	1:B:418:GLN:HG3	2.20	0.41
1:C:406:GLU:HG2	1:C:436:TYR:CE1	2.56	0.41
1:C:415:LYS:O	1:C:418:GLN:HG2	2.20	0.41
1:C:392:ASP:OD1	1:C:449:ASN:HB2	2.21	0.41
1:A:450:TYR:O	1:A:456:VAL:HG12	2.22	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	155/183 (85%)	150 (97%)	4 (3%)	1 (1%)	25	47
1	B	162/183 (88%)	156 (96%)	6 (4%)	0	100	100
1	C	164/183 (90%)	157 (96%)	6 (4%)	1 (1%)	25	47
All	All	481/549 (88%)	463 (96%)	16 (3%)	2 (0%)	34	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	401	PRO
1	A	328	PRO

### 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	135/158 (85%)	114 (84%)	21 (16%)	2	4
1	B	142/158 (90%)	113 (80%)	29 (20%)	1	2
1	C	147/158 (93%)	122 (83%)	25 (17%)	2	3
All	All	424/474 (90%)	349 (82%)	75 (18%)	2	3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	GLU
1	A	299	LEU
1	A	304	VAL
1	A	319	ARG
1	A	322	GLN
1	A	327	LYS
1	A	355	ASN
1	A	368	ARG
1	A	378	LEU
1	A	385	ARG
1	A	406	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	407	THR
1	A	418	GLN
1	A	422	THR
1	A	432	LEU
1	A	443	GLN
1	A	446	ARG
1	A	448	ARG
1	A	459	ARG
1	A	464	LEU
1	A	465	PRO
1	B	298	GLU
1	B	299	LEU
1	B	302	LEU
1	B	304	VAL
1	B	310	LEU
1	B	325	LYS
1	B	332	CYS
1	B	334	SER
1	B	341	LYS
1	B	368	ARG
1	B	378	LEU
1	B	394	SER
1	B	405	THR
1	B	407	THR
1	B	412	PRO
1	B	415	LYS
1	B	418	GLN
1	B	419	LYS
1	B	422	THR
1	B	424	ARG
1	B	427	LEU
1	B	443	GLN
1	B	444	ASP
1	B	446	ARG
1	B	447	LYS
1	B	456	VAL
1	B	459	ARG
1	B	463	GLU
1	B	465	PRO
1	C	292	LEU
1	C	293	GLN
1	C	295	LEU

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Mol	Chain	Res	Type
1	C	297	ARG
1	C	320	ARG
1	C	322	GLN
1	C	329	ASN
1	C	359	GLU
1	C	368	ARG
1	C	374	PHE
1	C	378	LEU
1	C	385	ARG
1	C	400	LYS
1	C	406	GLU
1	C	407	THR
1	C	418	GLN
1	C	419	LYS
1	C	432	LEU
1	C	440	ILE
1	C	443	GLN
1	C	446	ARG
1	C	447	LYS
1	C	453	ASP
1	C	467	LEU
1	C	471	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	402	GLN
1	A	443	GLN
1	B	418	GLN
1	C	329	ASN
1	C	449	ASN

### 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 carbohydrates 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, 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	159/183 (86%)	-0.45	0 <b>100</b> <b>100</b>	29, 43, 58, 74	0
1	B	166/183 (90%)	-0.40	2 (1%) <b>79</b> <b>76</b>	30, 46, 69, 88	0
1	C	170/183 (92%)	-0.29	2 (1%) <b>79</b> <b>76</b>	27, 45, 67, 82	0
All	All	495/549 (90%)	-0.38	4 (0%) <b>86</b> <b>84</b>	27, 44, 66, 88	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	4.1
1	C	295	LEU	4.1
1	C	293	GLN	2.2
1	B	307	ASP	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.