



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:09 PM UTC

PDB ID : 4M4E / pdb_00004m4e
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

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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

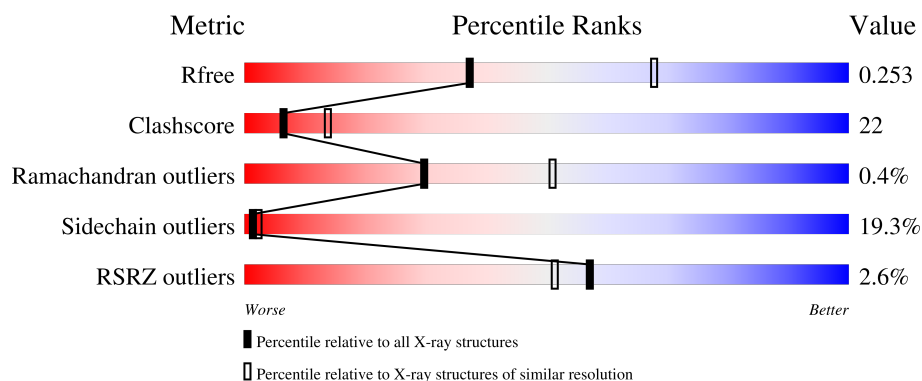
1 Overall quality at a glance

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	183	2% 45% 33% 8% 13%
1	B	183	4% 40% 35% 14% 9%
1	C	183	% 45% 37% 10% 7%

2 Entry composition

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
1	A	159	Total	C	N	O	S	0	0	0
			1279	827	222	229	1			
1	B	166	Total	C	N	O	S	0	0	0
			1338	861	233	243	1			
1	C	170	Total	C	N	O	S	0	0	0
			1390	893	251	245	1			

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

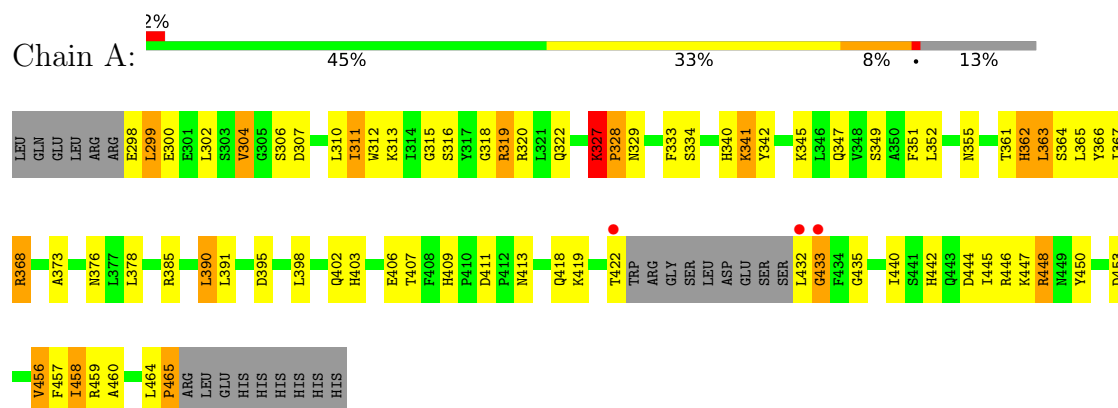
- Molecule 2 is water.

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

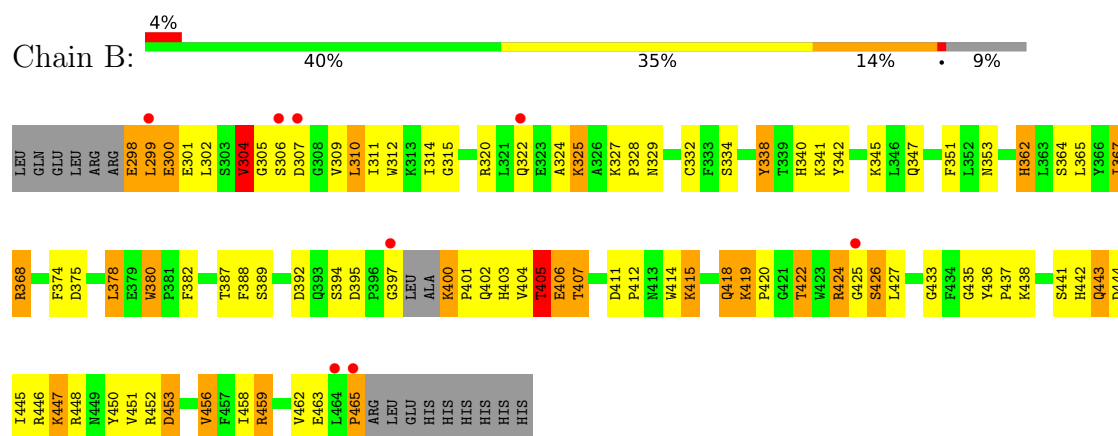
3 Residue-property plots

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.

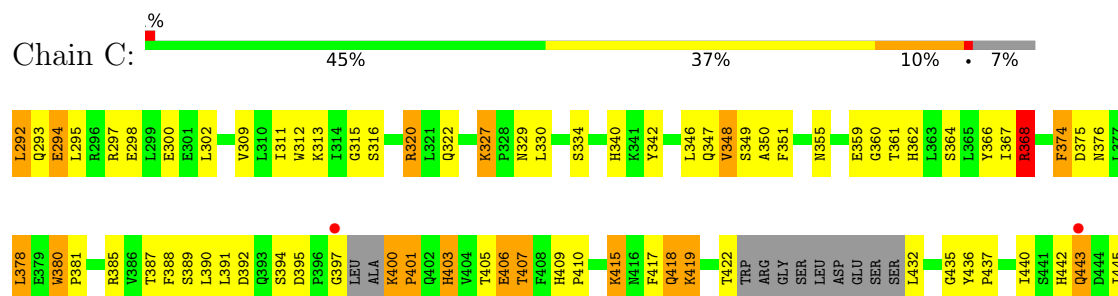
• Molecule 1: TNF receptor-associated factor 4



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R446	K447	R448	N449	Y450	D453	V456	F457	I458	R459	V462	L467	E468	H469	H470	R471	H472	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.30Å 88.20Å 118.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.03 – 2.60 36.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.1 (36.03-2.60) 93.1 (36.03-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.25 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.200 , 0.277 0.219 , 0.253	Depositor DCC
R_{free} test set	1846 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4096	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage'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.*

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 ⓘ

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	1.64	15/1317 (1.1%)	1.08	6/1784 (0.3%)
1	B	1.58	13/1378 (0.9%)	1.09	4/1866 (0.2%)
1	C	1.61	11/1431 (0.8%)	1.13	7/1934 (0.4%)
All	All	1.61	39/4126 (0.9%)	1.10	17/5584 (0.3%)

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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	469	HIS	CA-C	-7.06	1.44	1.52
1	B	380	TRP	CA-C	-6.41	1.46	1.52
1	C	340	HIS	CD2-NE2	-6.17	1.31	1.37
1	B	338	TYR	C-O	-6.10	1.16	1.23
1	B	426	SER	C-O	-5.98	1.19	1.24
1	A	442	HIS	CG-ND1	-5.90	1.31	1.38
1	B	309	VAL	C-O	-5.90	1.17	1.24
1	B	403	HIS	CD2-NE2	-5.87	1.31	1.37
1	A	362	HIS	CG-ND1	-5.85	1.31	1.38
1	B	362	HIS	CG-ND1	-5.84	1.31	1.38
1	A	340	HIS	CG-ND1	-5.64	1.32	1.38
1	A	460	ALA	C-O	-5.57	1.17	1.24
1	B	382	PHE	C-O	-5.50	1.17	1.24
1	B	442	HIS	CG-ND1	-5.49	1.32	1.38
1	A	311	ILE	C-O	-5.48	1.18	1.24
1	C	340	HIS	CG-ND1	-5.47	1.32	1.38
1	A	403	HIS	CG-ND1	-5.46	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	403	HIS	CG-ND1	-5.43	1.32	1.38
1	A	403	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	465	PRO	N-CD	5.37	1.55	1.47
1	C	309	VAL	C-O	-5.36	1.18	1.24
1	A	465	PRO	N-CD	5.32	1.55	1.47
1	C	409	HIS	CG-ND1	-5.28	1.32	1.38
1	A	362	HIS	CD2-NE2	-5.27	1.32	1.37
1	C	409	HIS	CD2-NE2	-5.27	1.32	1.37
1	B	462	VAL	C-O	-5.22	1.18	1.24
1	A	328	PRO	N-CD	5.21	1.55	1.47
1	A	409	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	409	HIS	CG-ND1	-5.16	1.32	1.38
1	C	403	HIS	CG-ND1	-5.12	1.32	1.38
1	C	442	HIS	CG-ND1	-5.10	1.32	1.38
1	C	380	TRP	NE1-CE2	-5.10	1.31	1.37
1	B	458	ILE	C-O	-5.10	1.18	1.24
1	B	340	HIS	CD2-NE2	-5.08	1.32	1.37
1	A	456	VAL	C-O	-5.08	1.19	1.24
1	A	458	ILE	C-O	-5.06	1.18	1.24
1	C	471	HIS	CG-ND1	-5.05	1.32	1.38
1	C	462	VAL	C-O	-5.05	1.17	1.24
1	A	373	ALA	C-O	-5.00	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	GLU	N-CA-C	7.77	119.39	111.07
1	A	341	LYS	N-CA-C	6.55	118.08	111.07
1	A	340	HIS	N-CA-C	-6.24	100.13	108.74
1	B	300	GLU	N-CA-C	5.81	117.69	111.36
1	C	443	GLN	N-CA-C	5.70	117.58	111.36
1	C	348	VAL	N-CA-C	5.41	117.10	108.87
1	C	415	LYS	N-CA-C	5.37	117.89	111.71
1	B	367	ILE	N-CA-C	5.36	115.83	108.12
1	C	327	LYS	N-CA-C	5.29	121.50	109.81
1	B	405	THR	N-CA-C	5.29	118.07	109.24
1	C	368	ARG	N-CA-C	5.27	118.16	109.72
1	B	433	GLY	N-CA-C	5.27	121.83	112.55
1	A	390	LEU	N-CA-C	-5.20	100.70	109.07
1	A	433	GLY	N-CA-C	5.13	120.42	111.50
1	C	360	GLY	N-CA-C	-5.12	108.98	115.08
1	A	327	LYS	CA-C-N	-5.09	113.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	327	LYS	C-N-CA	-5.09	113.47	119.84

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	69	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	173	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 (173) 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:HH11	1:A:368:ARG:HG2	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	0.91
1:B:300:GLU:OE2	1:B:345:LYS:NZ	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:H	1:B:299:LEU:HD13	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:C:361:THR:HG1	1:C:362:HIS:CE1	2.01	0.78
1:B:298:GLU:HB2	1:B:299:LEU:HD13	1.66	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
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:341:LYS:NZ	1:B:306:SER:HB2	2.11	0.64
1:A:368:ARG:HG2	1:A:368:ARG:NH1	1.98	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:A:402:GLN:CD	1:A:448:ARG:NH1	2.58	0.62
1:C:327:LYS:O	1:C:327:LYS:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:HH11	1:A:368:ARG:CG	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:C:395:ASP:C	1:C:397:GLY:H	2.16	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:380:TRP:HA	1:C:381:PRO:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:300:GLU:CD	1:B:345:LYS:HZ3	2.09	0.49
1:C:400:LYS:HE3	1:C:400:LYS:CA	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
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:443:GLN:H	1:B:443:GLN:CD	2.22	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:C:471:HIS:C	1:C:471:HIS:ND1	2.73	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:HH11	1:C:320:ARG:HG2	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: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:C:375:ASP:HA	1:C:378:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	2.01	0.43
1:B:415:LYS:HA	1:B:418:GLN:HE21	1.82	0.43
1:B:453:ASP:OD1	1:B:453:ASP:N	2.51	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
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:HD12	1:C:330:LEU:HA	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:C:415:LYS:HD2	1:C:418:GLN:HG3	2.00	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:NH1	1:A:368:ARG:CG	2.72	0.41
1:B:415:LYS:O	1:B:418:GLN:HG3	2.20	0.41
1:C:392:ASP:OD1	1:C:449:ASN:HB2	2.21	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: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%)	21	42
1	B	162/183 (88%)	156 (96%)	6 (4%)	0	100	100
1	C	164/183 (90%)	157 (96%)	6 (4%)	1 (1%)	21	42
All	All	481/549 (88%)	463 (96%)	16 (3%)	2 (0%)	30	51

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%)	112 (83%)	23 (17%)	2	4
1	B	142/158 (90%)	109 (77%)	33 (23%)	1	1
1	C	147/158 (93%)	121 (82%)	26 (18%)	2	3
All	All	424/474 (90%)	342 (81%)	82 (19%)	1	2

All (82) 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	327	LYS
1	A	355	ASN
1	A	363	LEU
1	A	368	ARG
1	A	378	LEU
1	A	385	ARG
1	A	406	GLU
1	A	407	THR
1	A	418	GLN
1	A	419	LYS
1	A	422	THR
1	A	432	LEU
1	A	440	ILE
1	A	445	ILE
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	322	GLN
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	400	LYS
1	B	405	THR
1	B	406	GLU
1	B	407	THR
1	B	415	LYS
1	B	418	GLN
1	B	419	LYS

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Mol	Chain	Res	Type
1	B	422	THR
1	B	424	ARG
1	B	426	SER
1	B	427	LEU
1	B	443	GLN
1	B	446	ARG
1	B	447	LYS
1	B	451	VAL
1	B	453	ASP
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
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	445	ILE
1	C	446	ARG
1	C	447	LYS
1	C	453	ASP
1	C	459	ARG
1	C	467	LEU
1	C	471	HIS

Sometimes 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	B	418	GLN
1	C	329	ASN
1	C	353	ASN
1	C	443	GLN

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	159/183 (86%)	0.12	3 (1%) 66 61	29, 43, 58, 74	0
1	B	166/183 (90%)	0.21	8 (4%) 35 30	30, 46, 69, 88	0
1	C	170/183 (92%)	0.11	2 (1%) 76 73	27, 45, 67, 82	0
All	All	495/549 (90%)	0.15	13 (2%) 57 51	27, 44, 66, 88	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	LEU	5.3
1	B	307	ASP	3.8
1	B	464	LEU	3.5
1	A	433	GLY	3.2
1	B	397	GLY	3.1
1	C	397	GLY	3.0
1	A	432	LEU	2.7
1	B	465	PRO	2.7
1	A	422	THR	2.4
1	B	425	GLY	2.2
1	B	306	SER	2.2
1	C	443	GLN	2.0
1	B	322	GLN	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 oligosaccharides 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.