W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 08:05 PM EDT

PDB ID	:	1D00
Title	:	STRUCTURE OF TNF RECEPTOR ASSOCIATED FACTOR 2 IN COMPLEX WITH A 5-RESIDUE CD40 PEPTIDE
Authors	:	Ye, H.; Park, Y.C.; Kreishman, M.; Kieff, E.; Wu, H.
Deposited on	:	1999-09-07
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

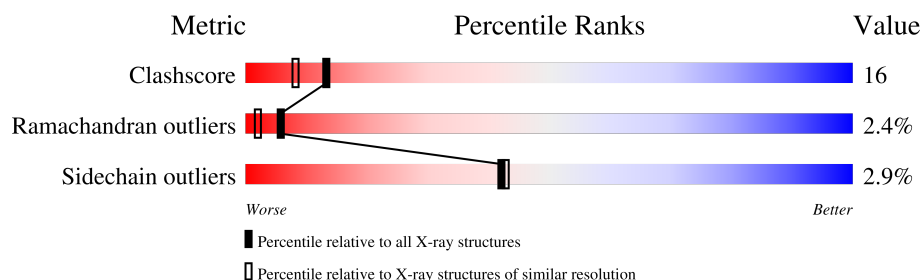|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		2.4%
Sidechain outliers		2.9%

Worse — *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	168	73% ... 23% ... •
1	B	168	70% ... 26% ... •
1	C	168	74% ... 23% ... •
1	D	168	73% ... 25% ... •
1	E	168	74% ... 22% ... •
1	F	168	70% ... 27% ... •
1	G	168	71% ... 27% ... •
1	H	168	68% ... 29% ... •

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Mol	Chain	Length	Quality of chain
2	I	7	71% 14% 14%
2	J	7	43% 57%
2	K	7	57% 43%
2	L	7	71% 29%
2	M	7	71% 29%
2	N	7	71% 29%
2	O	7	71% 14% 14%
2	P	7	57% 43%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10670 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 TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	B	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	C	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	D	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	E	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	F	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	G	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			
1	H	168	Total	C	N	O	S	0	0	0
			1282	825	217	231	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	362	ALA	PRO	CONFLICT	GB 1363002
A	365	ARG	LEU	CONFLICT	GB 1363002
B	362	ALA	PRO	CONFLICT	GB 1363002
B	365	ARG	LEU	CONFLICT	GB 1363002
C	362	ALA	PRO	CONFLICT	GB 1363002
C	365	ARG	LEU	CONFLICT	GB 1363002
D	362	ALA	PRO	CONFLICT	GB 1363002
D	365	ARG	LEU	CONFLICT	GB 1363002
E	362	ALA	PRO	CONFLICT	GB 1363002
E	365	ARG	LEU	CONFLICT	GB 1363002
F	362	ALA	PRO	CONFLICT	GB 1363002
F	365	ARG	LEU	CONFLICT	GB 1363002

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Chain	Residue	Modelled	Actual	Comment	Reference
G	362	ALA	PRO	CONFLICT	GB 1363002
G	365	ARG	LEU	CONFLICT	GB 1363002
H	362	ALA	PRO	CONFLICT	GB 1363002
H	365	ARG	LEU	CONFLICT	GB 1363002

- Molecule 2 is a protein called B-CELL SURFACE ANTIGEN CD40.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	7	Total 43	C 26	N 7	O 10	0	0	1
2	J	7	Total 43	C 26	N 7	O 10	0	0	1
2	K	7	Total 43	C 26	N 7	O 10	0	0	1
2	L	7	Total 43	C 26	N 7	O 10	0	0	1
2	M	7	Total 43	C 26	N 7	O 10	0	0	1
2	N	7	Total 43	C 26	N 7	O 10	0	0	1
2	O	7	Total 43	C 26	N 7	O 10	0	0	1
2	P	7	Total 43	C 26	N 7	O 10	0	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total 12	O 12	0	0
3	B	3	Total 3	O 3	0	0
3	C	11	Total 11	O 11	0	0
3	D	7	Total 7	O 7	0	0
3	E	5	Total 5	O 5	0	0
3	F	9	Total 9	O 9	0	0
3	G	8	Total 8	O 8	0	0

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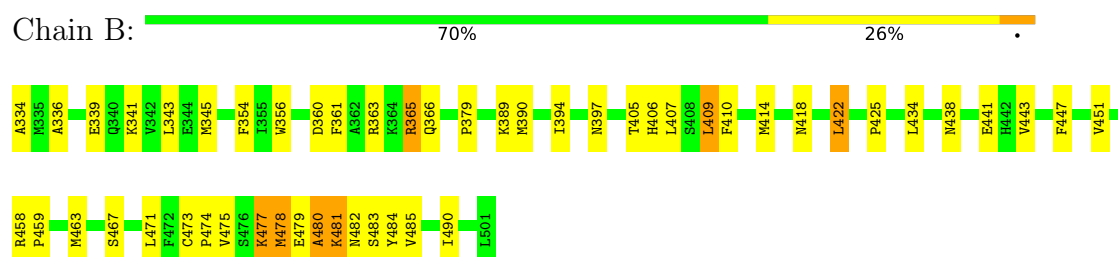| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	13	Total 13	O 13	0	0
3	K	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0

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. 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. 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.
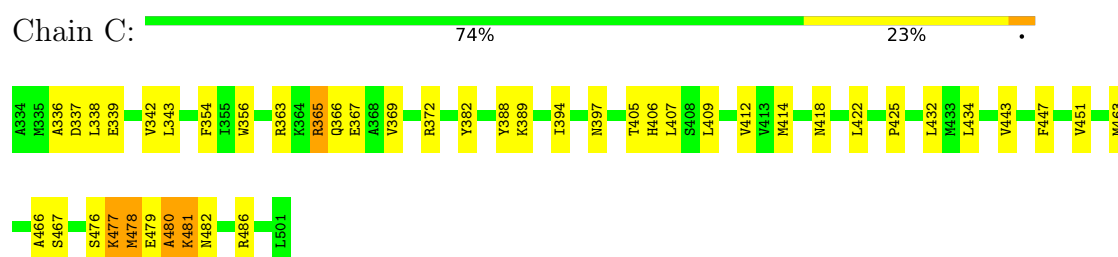
Note EDS was not executed.

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2
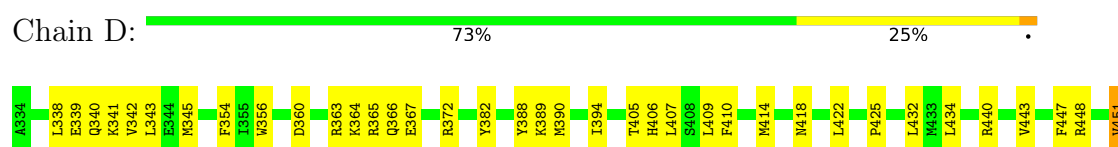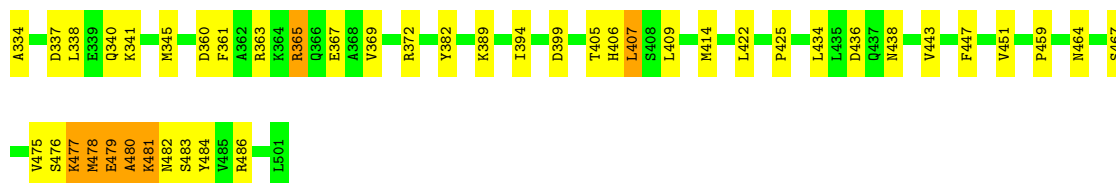
Chain A:

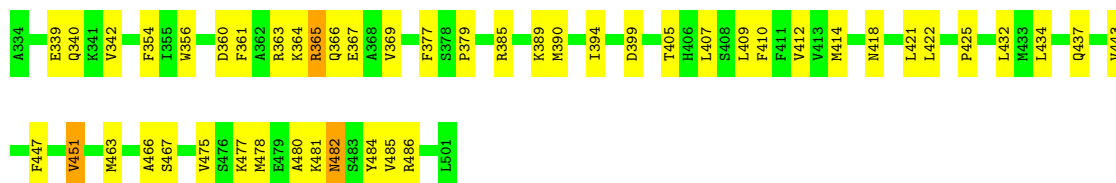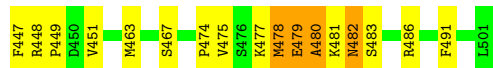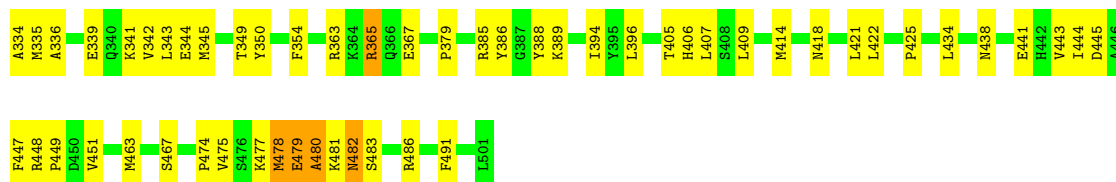• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain B:

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain C:

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain D:

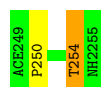F456 M463 S476 K477 M478 E479 A480 K481 N482 L501

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain E: 74% 22%

A334 D337 L338 E339 Q340 K341 M345 D360 F361 A362 R363 K364 R365 Q366 E367 A368 V369 R372 Y382 K389 I394 D399 T405 H406 L407 S408 L409 M414 L422 P425 L434 L435 D436 Q437 N438 V443 F447 V451 P459 N464 S467

V475 S476 K477 M478 E479 A480 K481 N482 S483 Y484 V485 R486 L501

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain F: 70% 27%

A334 M335 A336 D337 L338 E339 Q340 K341 V342 L343 I355 D360 F361 R365 Q366 K389 R393 I394 N397 T405 H406 L407 S408 L409 V412 V413 M414 L422 P425 Q428 M433 L434 R440 V443 I444 D445 A446 F447 R448 V451 A466 C469 P470

C473 P474 K477 M478 E479 A480 K481 N482 S483 Y484 V485 R486 I490 F491 D497 L501

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain G: 71% 27%

A334 E339 Q340 K341 V342 F354 I355 W356 D360 F361 A362 R363 K364 R365 Q366 E367 A368 V369 F377 S378 P379 R385 K389 M390 I394 D399 T405 H406 L407 S408 L409 F410 F411 V412 V413 M414 N418 L421 L422 P425 L432 M433 L434 Q437 V443

F447 V451 M463 A466 S467 V475 S476 K477 M478 E479 A480 K481 N482 S483 Y484 V485 R486 L501

• Molecule 1: TUMOR NECROSIS FACTOR RECEPTOR ASSOCIATED PROTEIN 2

Chain H: 68% 29%

A334 M335 A336 E339 Q340 K341 V342 L343 E344 M345 T349 Y350 F354 R363 K364 R365 Q366 E367 P379 R385 Y386 G387 Y388 K389 I394 Y395 L396 T405 H406 L407 S408 L409 M414 N418 L421 L422 P425 L434 N438 E441 H442 V443 I444 D445 A446

F447 R448 P449 D450 V451 M463 S467 P474 V475 S476 K477 M478 E479 A480 K481 N482 S483 R486 F491 L501

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain I: 71% 14% 14%

ACE249 P250 T254 NH2255

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain J:

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain K:

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

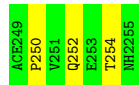Chain L:

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain M:
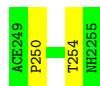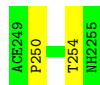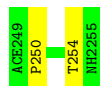

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain N:

• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain O:
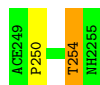
• Molecule 2: B-CELL SURFACE ANTIGEN CD40

Chain P:

4 Data and refinement statistics ⓘ

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, α, β, γ	111.40Å 111.40Å 111.40Å 103.70° 103.70° 103.70°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10670	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2

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	0.44	0/1312	0.71	0/1781
1	B	0.42	0/1312	0.71	0/1781
1	C	0.43	0/1312	0.72	0/1781
1	D	0.44	0/1312	0.71	0/1781
1	E	0.43	0/1312	0.70	1/1781 (0.1%)
1	F	0.44	0/1312	0.73	1/1781 (0.1%)
1	G	0.42	0/1312	0.71	0/1781
1	H	0.41	0/1312	0.71	0/1781
2	I	0.42	0/40	0.74	0/55
2	J	0.51	0/40	0.77	0/55
2	K	0.47	0/40	0.69	0/55
2	L	0.48	0/40	0.81	0/55
2	M	0.44	0/40	0.73	0/55
2	N	0.47	0/40	0.73	0/55
2	O	0.49	0/40	0.71	0/55
2	P	0.50	0/40	0.79	0/55
All	All	0.43	0/10816	0.71	2/14688 (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	E	407	LEU	N-CA-C	-5.20	96.96	111.00
1	F	407	LEU	N-CA-C	-5.15	97.09	111.00

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	1282	0	1242	36	0
1	B	1282	0	1242	45	0
1	C	1282	0	1242	37	0
1	D	1282	0	1242	43	0
1	E	1282	0	1242	41	0
1	F	1282	0	1242	43	0
1	G	1282	0	1242	44	0
1	H	1282	0	1242	53	0
2	I	43	0	40	3	0
2	J	43	0	40	7	0
2	K	43	0	40	6	0
2	L	43	0	40	1	0
2	M	43	0	40	3	0
2	N	43	0	40	1	0
2	O	43	0	40	4	0
2	P	43	0	40	9	0
3	A	12	0	0	1	0
3	B	3	0	0	0	0
3	C	11	0	0	0	0
3	D	7	0	0	3	0
3	E	5	0	0	1	0
3	F	9	0	0	4	0
3	G	8	0	0	0	0
3	H	13	0	0	5	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	10670	0	10256	337	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 16.

The worst 5 of 337 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:H:425:PRO:HG3	1:H:451:VAL:HG13	1.41	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:PRO:HG3	1:A:451:VAL:HG13	1.43	0.99
1:H:394:ILE:HD11	1:H:407:LEU:HD21	1.41	0.99
1:G:389:LYS:HG2	1:G:414:MET:HE3	1.46	0.95
1:E:425:PRO:HG3	1:E:451:VAL:HG13	1.51	0.93

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	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	6	2
1	B	166/168 (99%)	156 (94%)	6 (4%)	4 (2%)	6	2
1	C	166/168 (99%)	154 (93%)	7 (4%)	5 (3%)	4	1
1	D	166/168 (99%)	156 (94%)	7 (4%)	3 (2%)	8	3
1	E	166/168 (99%)	155 (93%)	5 (3%)	6 (4%)	3	1
1	F	166/168 (99%)	158 (95%)	5 (3%)	3 (2%)	8	3
1	G	166/168 (99%)	155 (93%)	9 (5%)	2 (1%)	13	7
1	H	166/168 (99%)	152 (92%)	8 (5%)	6 (4%)	3	1
2	I	5/7 (71%)	5 (100%)	0	0	100	100
2	J	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	K	5/7 (71%)	5 (100%)	0	0	100	100
2	L	5/7 (71%)	5 (100%)	0	0	100	100
2	M	5/7 (71%)	5 (100%)	0	0	100	100
2	N	5/7 (71%)	5 (100%)	0	0	100	100
2	O	5/7 (71%)	5 (100%)	0	0	100	100
2	P	5/7 (71%)	5 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1368/1400 (98%)	1281 (94%)	54 (4%)	33 (2%)	6 2

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	LYS
1	A	480	ALA
1	B	477	LYS
1	B	480	ALA
1	C	477	LYS

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	132/144 (92%)	128 (97%)	4 (3%)	41	41
1	B	132/144 (92%)	127 (96%)	5 (4%)	33	31
1	C	132/144 (92%)	130 (98%)	2 (2%)	65	69
1	D	132/144 (92%)	129 (98%)	3 (2%)	50	53
1	E	132/144 (92%)	129 (98%)	3 (2%)	50	53
1	F	132/144 (92%)	126 (96%)	6 (4%)	27	24
1	G	132/144 (92%)	129 (98%)	3 (2%)	50	53
1	H	132/144 (92%)	130 (98%)	2 (2%)	65	69
2	I	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	J	5/5 (100%)	5 (100%)	0	100	100
2	K	5/5 (100%)	5 (100%)	0	100	100
2	L	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	M	5/5 (100%)	5 (100%)	0	100	100
2	N	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	O	5/5 (100%)	4 (80%)	1 (20%)	1	0
2	P	5/5 (100%)	5 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1096/1192 (92%)	1064 (97%)	32 (3%)	42	43

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	254	THR
2	L	254	THR
1	D	366	GLN
1	D	365	ARG
2	N	254	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	406	HIS
1	G	438	ASN
1	G	406	HIS
1	G	461	ASN
1	C	461	ASN

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 monosaccharides 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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.