



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 05:15 PM BST

PDB ID : 4V46  
Title : Crystal structure of the BAFF-BAFF-R complex  
Authors : Kim, H.M.; Yu, K.S.; Lee, M.E.; Shin, D.R.; Kim, Y.S.; Paik, S.G.; Yoo, O.J.;  
Lee, H.; Lee, J.-O.  
Deposited on : 2003-03-23  
Resolution : 3.30 Å(reported)

This is a wwPDB validation summary 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 <http://wwpdb.org/ValidationPDFNotes.html>

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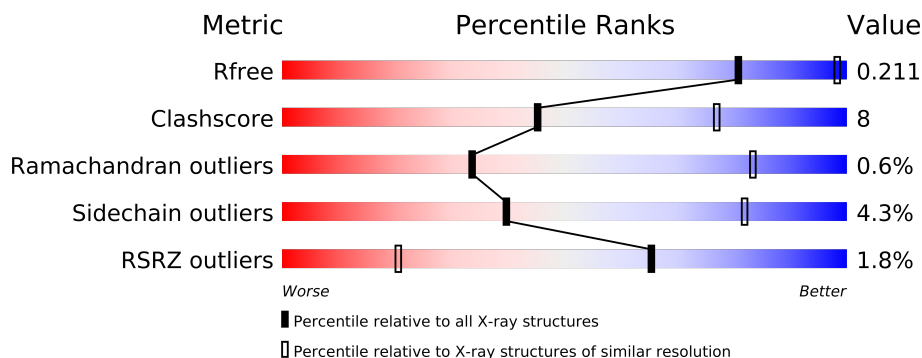
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A0	148	
1	A1	148	
1	A2	148	
1	A3	148	
1	A4	148	
1	A5	148	
1	A6	148	
1	A7	148	
1	A8	148	
1	A9	148	
1	AA	148	
1	AB	148	
1	AC	148	
1	AD	148	

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Mol	Chain	Length	Quality of chain
1	AE	148	
1	AF	148	
1	AG	148	
1	AH	148	
1	AI	148	
1	AJ	148	
1	AK	148	
1	AL	148	
1	AM	148	
1	AN	148	
1	AO	148	
1	AP	148	
1	AQ	148	
1	AR	148	
1	AS	148	
1	AT	148	
1	AU	148	
1	AV	148	
1	AW	148	
1	AX	148	
1	AY	148	
1	AZ	148	
1	Aa	148	
1	Ab	148	
1	Ac	148	
1	Ad	148	
1	Ae	148	
1	Af	148	
1	Ag	148	
1	Ah	148	
1	Ai	148	
1	Aj	148	
1	Ak	148	
1	Al	148	
1	Am	148	
1	An	148	
1	Ao	148	
1	Ap	148	
1	Aq	148	
1	Ar	148	
1	As	148	
1	At	148	

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Mol	Chain	Length	Quality of chain
1	Au	148	
1	Av	148	
1	Aw	148	
1	Ax	148	
2	B0	63	
2	B1	63	
2	B2	63	
2	B3	63	
2	B4	63	
2	B5	63	
2	B6	63	
2	B7	63	
2	B8	63	
2	B9	63	
2	BA	63	
2	BB	63	
2	BC	63	
2	BD	63	
2	BE	63	
2	BF	63	
2	BG	63	
2	BH	63	
2	BI	63	
2	BJ	63	
2	BK	63	
2	BL	63	
2	BM	63	
2	BN	63	
2	BO	63	
2	BP	63	
2	BQ	63	
2	BR	63	
2	BS	63	
2	BT	63	
2	BU	63	
2	BV	63	
2	BW	63	
2	BX	63	
2	BY	63	
2	BZ	63	
2	Ba	63	
2	Bb	63	

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Mol	Chain	Length	Quality of chain
2	Bc	63	
2	Bd	63	
2	Be	63	
2	Bf	63	
2	Bg	63	
2	Bh	63	
2	Bi	63	
2	Bj	63	
2	Bk	63	
2	Bl	63	
2	Bm	63	
2	Bn	63	
2	Bo	63	
2	Bp	63	
2	Bq	63	
2	Br	63	
2	Bs	63	
2	Bt	63	
2	Bu	63	
2	Bv	63	
2	Bw	63	
2	Bx	63	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A1	301	-	X
3	MG	A4	301	-	X
3	MG	A4	302	-	X
3	MG	A5	301	-	X
3	MG	A5	302	-	X
3	MG	A6	301	-	X
3	MG	A6	302	-	X
3	MG	A7	301	-	X
3	MG	A8	301	-	X
3	MG	A8	302	-	X
3	MG	A9	301	-	X
3	MG	A9	302	-	X
3	MG	AA	1001	-	X
3	MG	AA	1002	-	X
3	MG	AB	301	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MG	AC	301	-	X
3	MG	AD	301	-	X
3	MG	AF	301	-	X
3	MG	AJ	301	-	X
3	MG	AN	301	-	X
3	MG	AO	301	-	X
3	MG	AQ	301	-	X
3	MG	AQ	302	-	X
3	MG	AR	301	-	X
3	MG	Aa	301	-	X
3	MG	Ac	301	-	X
3	MG	Ac	302	-	X
3	MG	Ad	301	-	X
3	MG	Af	301	-	X
3	MG	Ah	301	-	X
3	MG	Ak	301	-	X
3	MG	Am	301	-	X
3	MG	An	301	-	X
3	MG	Ap	301	-	X
3	MG	Aq	301	-	X
3	MG	Ar	301	-	X
3	MG	As	301	-	X
3	MG	Av	301	-	X
3	MG	Aw	301	-	X
3	MG	Aw	302	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 79720 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ligand superfamily member 13B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AB	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AC	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AD	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AE	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AF	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AG	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AH	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AI	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AJ	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AK	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AL	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AM	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AN	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AO	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	AP	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AR	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AS	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AT	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AU	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AV	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AW	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AX	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AY	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	AZ	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A0	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A1	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A2	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A3	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A4	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A5	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A6	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A7	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A8	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	A9	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Aa	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Ab	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ac	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ad	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ae	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Af	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ag	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ah	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ai	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Aj	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ak	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Al	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Am	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	An	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ao	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ap	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Aq	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Ar	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	As	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	At	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Au	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0
1	Av	144	Total 1143	C 736	N 184	O 218	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Aw	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			
1	Ax	144	Total	C	N	O	S	0	0	0
			1143	736	184	218	5			

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 13C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BA	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BB	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BC	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BD	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BE	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BF	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BG	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BH	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BI	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BJ	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BK	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BL	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BM	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BN	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BO	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BP	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			
2	BQ	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BR	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BS	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BT	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BU	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BV	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BW	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BX	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BY	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	BZ	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B0	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B1	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B2	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B3	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B4	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B5	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B6	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B7	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B8	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	B9	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Ba	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bb	25	Total 185	C 118	N 33	O 30	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Bc	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bd	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Be	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bf	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bg	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bh	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bi	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bj	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bk	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bl	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bm	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bn	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bo	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bp	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bq	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Br	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bs	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bt	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bu	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bv	25	Total 185	C 118	N 33	O 30	S 4	0	0	0
2	Bw	25	Total 185	C 118	N 33	O 30	S 4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Bx	25	Total	C	N	O	S	0	0	0
			185	118	33	30	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Aq	1	Total	Mg	0	0
			1	1		
3	Ah	1	Total	Mg	0	0
			1	1		
3	AB	1	Total	Mg	0	0
			1	1		
3	Ac	2	Total	Mg	0	0
			2	2		
3	A6	2	Total	Mg	0	0
			2	2		
3	AN	1	Total	Mg	0	0
			1	1		
3	Af	1	Total	Mg	0	0
			1	1		
3	Ap	1	Total	Mg	0	0
			1	1		
3	AJ	1	Total	Mg	0	0
			1	1		
3	Ak	1	Total	Mg	0	0
			1	1		
3	Aw	2	Total	Mg	0	0
			2	2		
3	AA	2	Total	Mg	0	0
			2	2		
3	An	1	Total	Mg	0	0
			1	1		
3	A5	2	Total	Mg	0	0
			2	2		
3	AR	1	Total	Mg	0	0
			1	1		
3	As	1	Total	Mg	0	0
			1	1		
3	A1	1	Total	Mg	0	0
			1	1		
3	AD	1	Total	Mg	0	0
			1	1		

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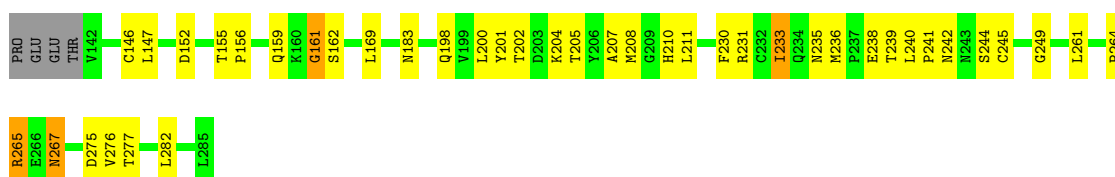
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Av	1	Total 1	Mg 1	0	0
3	Aa	1	Total 1	Mg 1	0	0
3	A4	2	Total 2	Mg 2	0	0
3	Ar	1	Total 1	Mg 1	0	0
3	A9	2	Total 2	Mg 2	0	0
3	Am	1	Total 1	Mg 1	0	0
3	AQ	2	Total 2	Mg 2	0	0
3	Ad	1	Total 1	Mg 1	0	0
3	AC	1	Total 1	Mg 1	0	0
3	A7	1	Total 1	Mg 1	0	0
3	A8	2	Total 2	Mg 2	0	0
3	AO	1	Total 1	Mg 1	0	0
3	AF	1	Total 1	Mg 1	0	0

### 3 Residue-property plots

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.

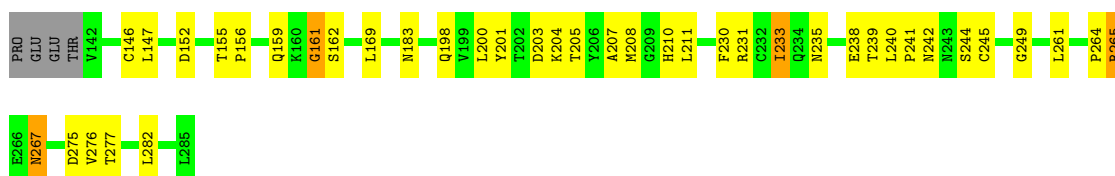
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AA: 



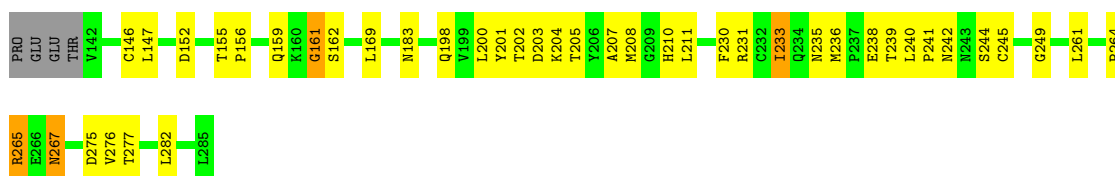
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AB: 



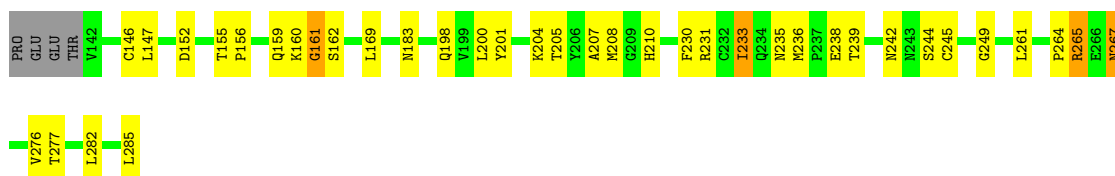
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AC: 



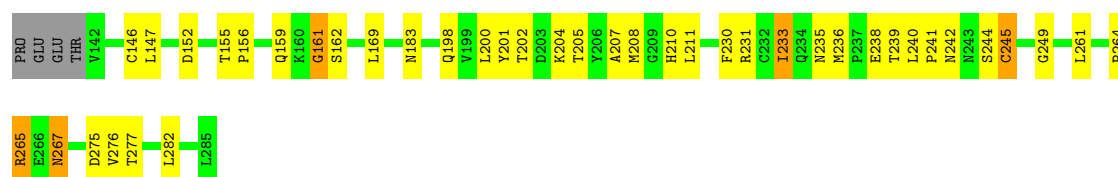
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AD: 



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AE: 



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AF:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AG:



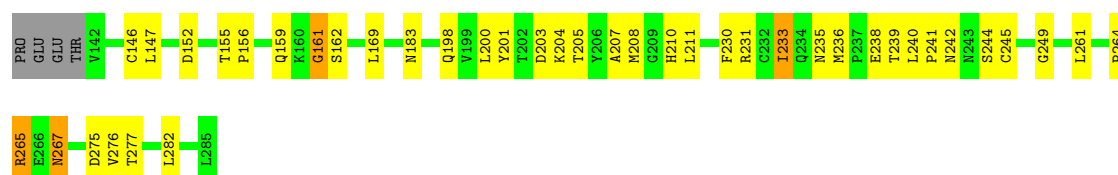
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AH:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AI:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

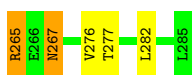
Chain AJ:





- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AK:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AL:



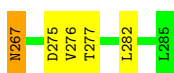
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AM:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AN:

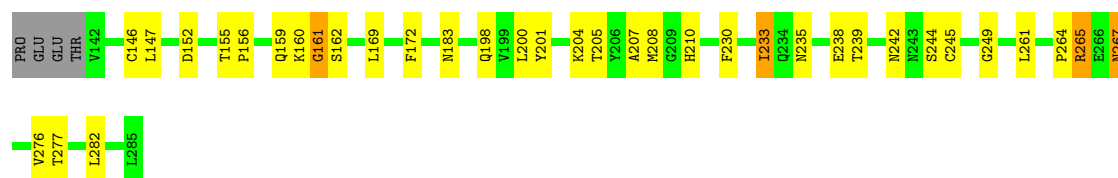


- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AO:



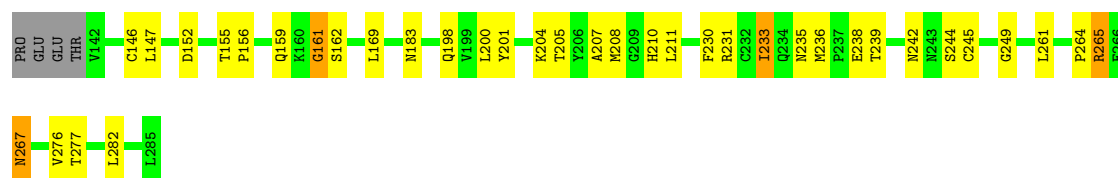
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AP: 

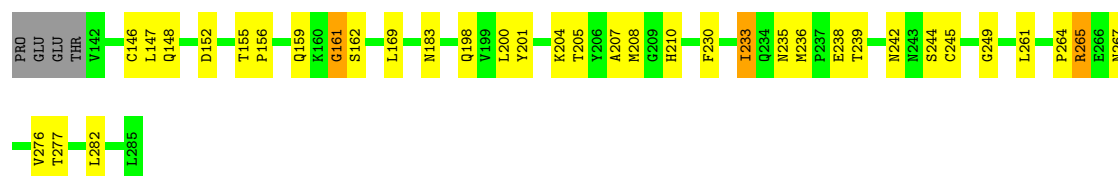
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AQ: 

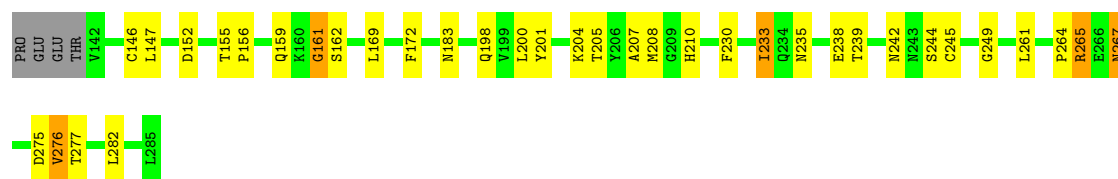
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AR: 

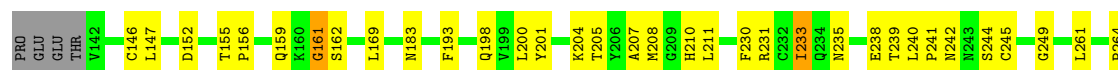
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AS: 

- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AT: 

- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AU: 



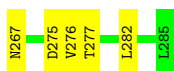
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AV:



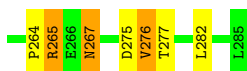
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AW:



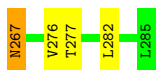
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AX:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AY:



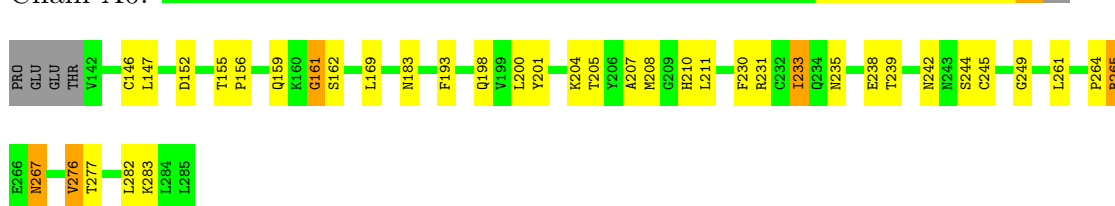
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AZ:



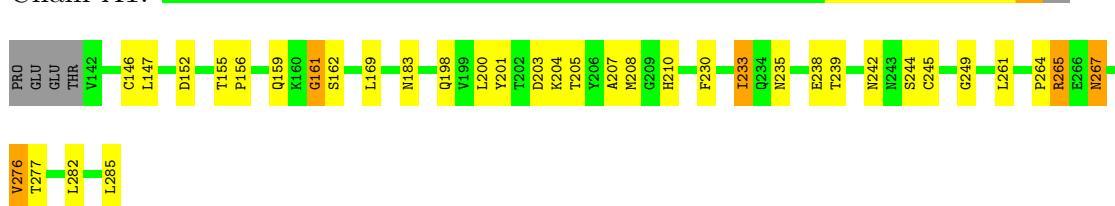
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A0:



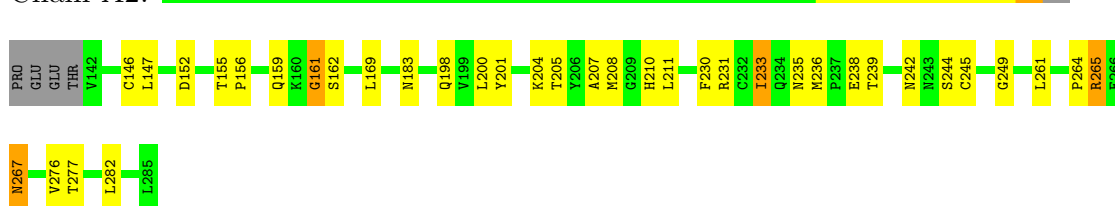
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A1:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A2:



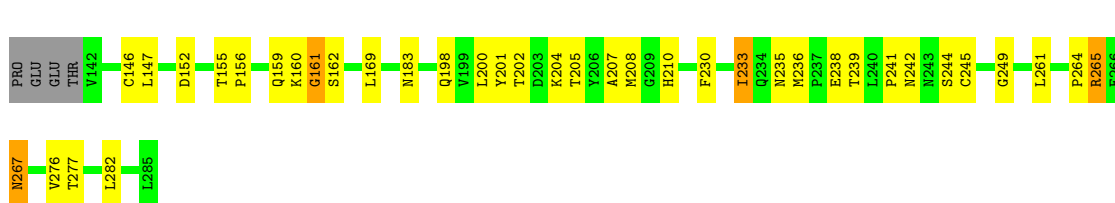
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A3:



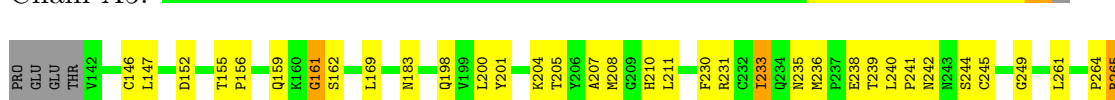
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A4:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

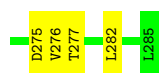
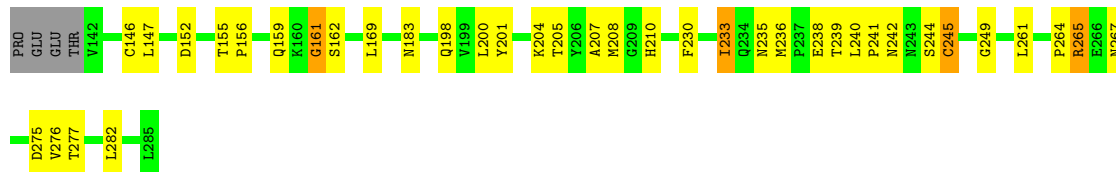
Chain A5:





- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A6:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A7:



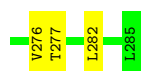
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A8:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A9:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Aa:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ab:



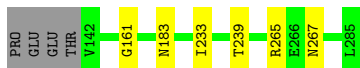
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ac:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ad:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ae:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Af:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ag:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ah:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ai:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Aj:



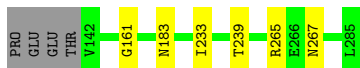
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ak:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Al:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Am:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain An:



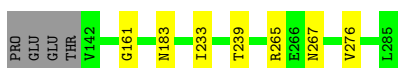
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ao:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ap:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Aq:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ar:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain As:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain At:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Au:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Av:



- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Aw:



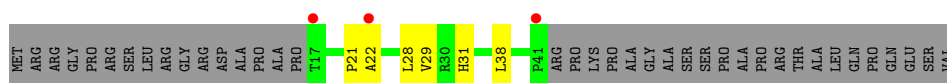
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ax:



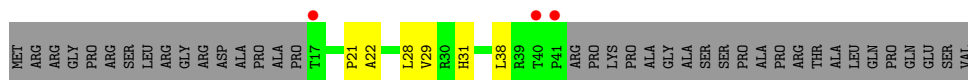
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BA:



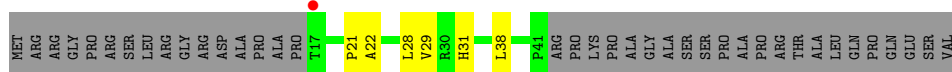
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BB:



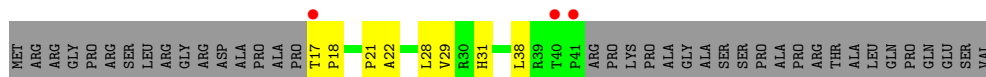
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BC:



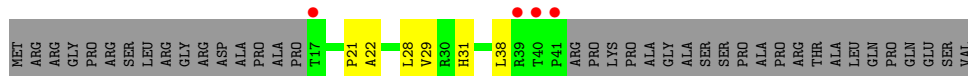
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BD:



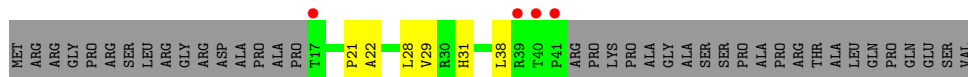
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BE:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BF:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BG:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BH:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BI:



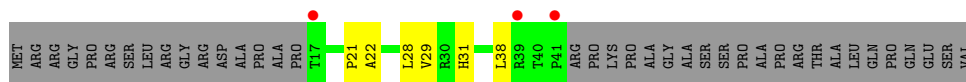
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BJ: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BK: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BL: 



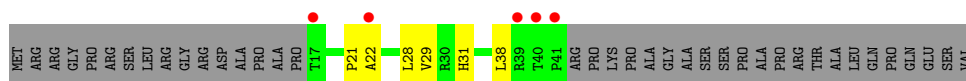
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BM: 



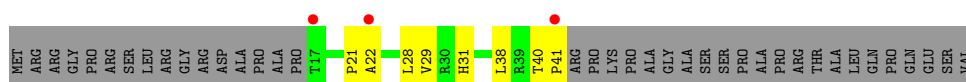
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BN: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BO: 



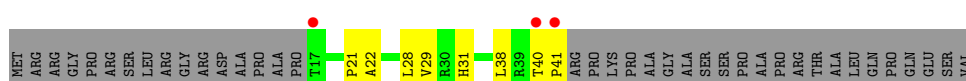
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BP: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BQ: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BR: 



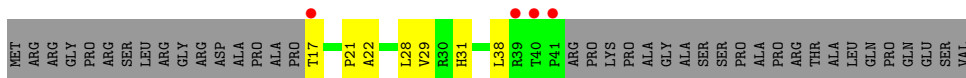
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BS: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BT: 



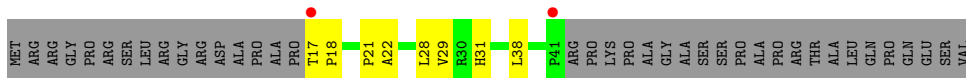
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BU: 



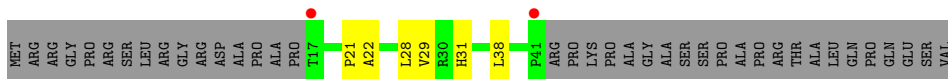
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BV: 



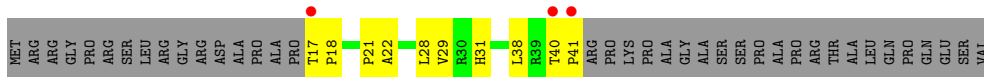
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BW: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BX: 



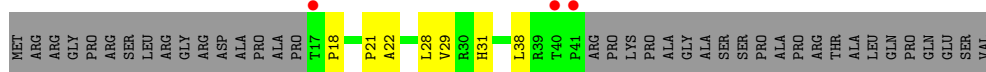
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BY: 



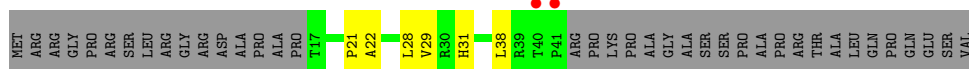
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BZ:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B0:



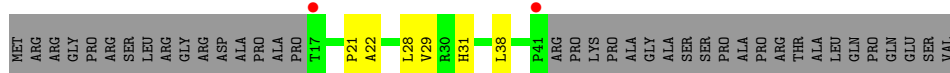
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B1:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B2:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B3:



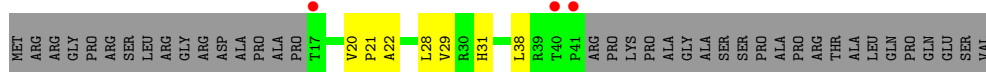
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B4:



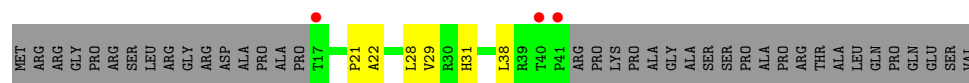
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B5:



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B6: 



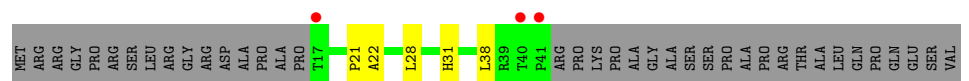
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B7: 



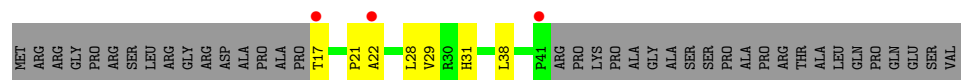
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B8: 



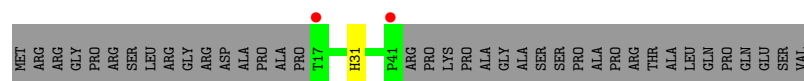
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain B9: 



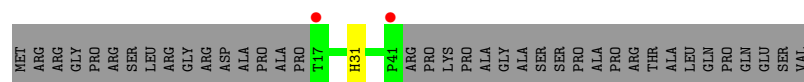
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Ba: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bb: 



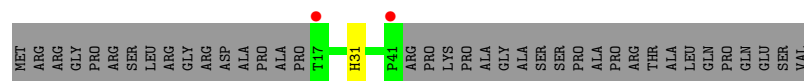
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bc: 



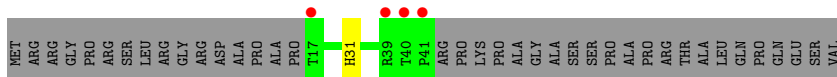
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bd: 



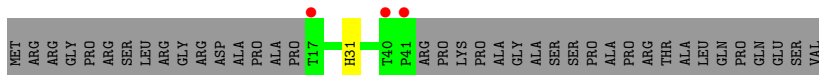
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Be: 



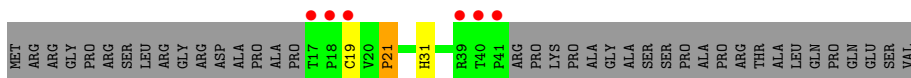
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bf: 



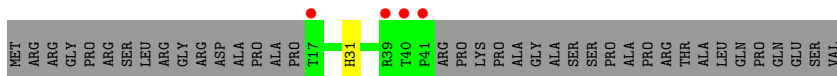
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bg: 



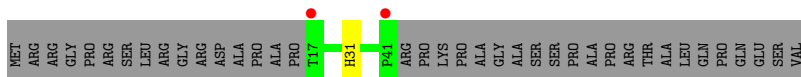
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bh: 



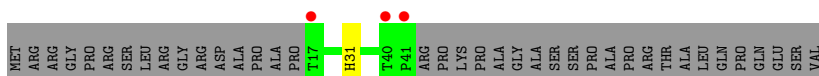
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bi: 



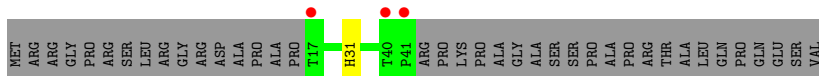
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bj: 



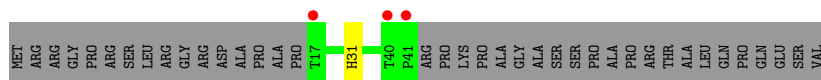
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bk: 



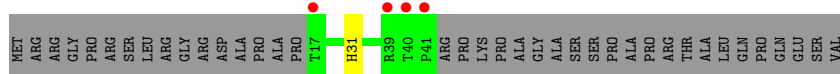
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bl: 



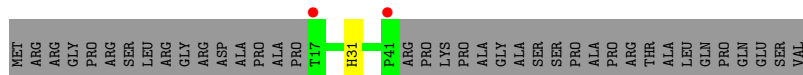
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bm:



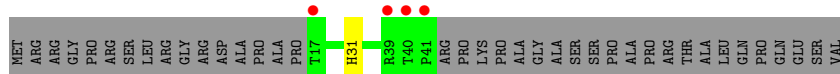
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bn:



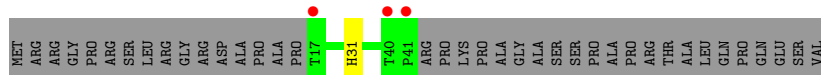
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bo:



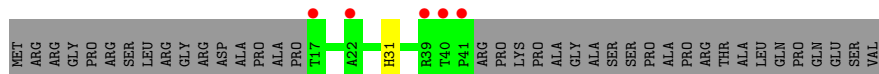
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bp:



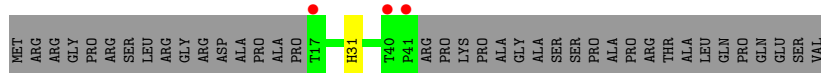
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bq:



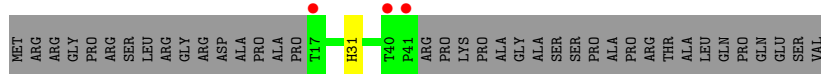
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Br:



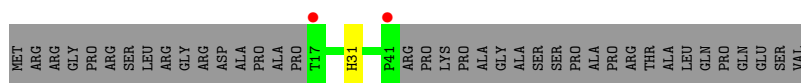
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bs:



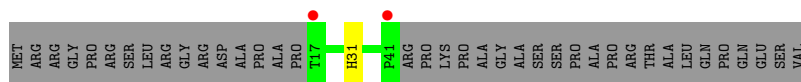
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bt: 



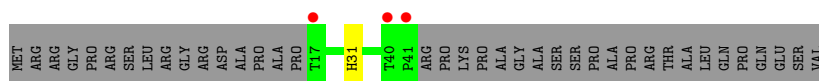
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bu: 



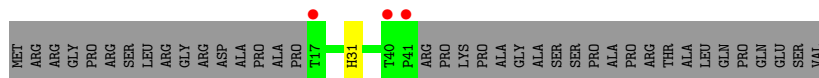
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bv: 



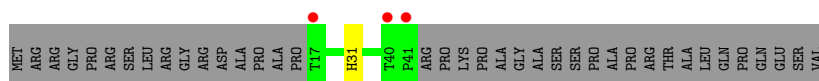
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bw: 



- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain Bx: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.50Å 194.80Å 274.40Å 90.00° 93.30° 90.00°	Depositor
Resolution (Å)	19.95 – 3.30 19.92 – 3.27	Depositor EDS
% Data completeness (in resolution range)	93.4 (19.95-3.30) 92.4 (19.92-3.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.226 0.205 , 0.211	Depositor DCC
$R_{free}$ test set	12736 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 4.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	6 of 276000 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	79720	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	A0	0.51	0/1165	0.64	0/1574
1	A1	0.53	0/1165	0.64	0/1574
1	A2	0.52	0/1165	0.64	0/1574
1	A3	0.56	0/1165	0.64	0/1574
1	A4	0.53	0/1165	0.65	0/1574
1	A5	0.54	0/1165	0.64	0/1574
1	A6	0.50	0/1165	0.65	0/1574
1	A7	0.52	0/1165	0.65	0/1574
1	A8	0.51	0/1165	0.64	0/1574
1	A9	0.52	0/1165	0.64	0/1574
1	AA	0.53	0/1165	0.66	0/1574
1	AB	0.51	0/1165	0.64	0/1574
1	AC	0.51	0/1165	0.64	0/1574
1	AD	0.56	0/1165	0.64	0/1574
1	AE	0.50	0/1165	0.65	0/1574
1	AF	0.53	0/1165	0.64	0/1574
1	AG	0.53	0/1165	0.65	0/1574
1	AH	0.51	0/1165	0.64	0/1574
1	AI	0.51	0/1165	0.65	0/1574
1	AJ	0.56	0/1165	0.64	0/1574
1	AK	0.50	0/1165	0.64	0/1574
1	AL	0.55	0/1165	0.64	0/1574
1	AM	0.53	0/1165	0.66	0/1574
1	AN	0.53	0/1165	0.64	0/1574
1	AO	0.52	0/1165	0.65	0/1574
1	AP	0.56	0/1165	0.64	0/1574
1	AQ	0.50	0/1165	0.65	0/1574
1	AR	0.53	0/1165	0.65	0/1574
1	AS	0.51	0/1165	0.65	0/1574
1	AT	0.52	0/1165	0.64	0/1574
1	AU	0.51	0/1165	0.64	0/1574
1	AV	0.53	0/1165	0.64	0/1574

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AW	0.50	0/1165	0.65	0/1574
1	AX	0.53	0/1165	0.65	0/1574
1	AY	0.54	0/1165	0.66	0/1574
1	AZ	0.53	0/1165	0.64	0/1574
1	Aa	0.52	0/1165	0.64	0/1574
1	Ab	0.54	0/1165	0.64	0/1574
1	Ac	0.51	0/1165	0.65	0/1574
1	Ad	0.55	0/1165	0.64	0/1574
1	Ae	0.51	0/1165	0.64	0/1574
1	Af	0.52	0/1165	0.65	0/1574
1	Ag	0.52	0/1165	0.65	0/1574
1	Ah	0.54	0/1165	0.64	0/1574
1	Ai	0.51	0/1165	0.64	0/1574
1	Aj	0.55	0/1165	0.64	0/1574
1	Ak	0.50	0/1165	0.65	0/1574
1	Al	0.50	0/1165	0.64	0/1574
1	Am	0.51	0/1165	0.64	0/1574
1	An	0.54	0/1165	0.64	0/1574
1	Ao	0.52	0/1165	0.66	0/1574
1	Ap	0.57	0/1165	0.64	0/1574
1	Aq	0.51	0/1165	0.65	0/1574
1	Ar	0.51	0/1165	0.64	0/1574
1	As	0.52	0/1165	0.65	0/1574
1	At	0.54	0/1165	0.64	0/1574
1	Au	0.51	0/1165	0.64	0/1574
1	Av	0.53	0/1165	0.64	0/1574
1	Aw	0.54	0/1165	0.64	0/1574
1	Ax	0.53	0/1165	0.64	0/1574
2	B0	0.46	0/189	0.63	0/259
2	B1	0.44	0/189	0.64	0/259
2	B2	0.44	0/189	0.65	0/259
2	B3	0.44	0/189	0.64	0/259
2	B4	0.46	0/189	0.63	0/259
2	B5	0.50	0/189	0.65	0/259
2	B6	0.44	0/189	0.63	0/259
2	B7	0.45	0/189	0.64	0/259
2	B8	0.45	0/189	0.63	0/259
2	B9	0.44	0/189	0.64	0/259
2	BA	0.57	0/189	0.65	0/259
2	BB	0.44	0/189	0.63	0/259
2	BC	0.45	0/189	0.65	0/259
2	BD	0.47	0/189	0.66	0/259
2	BE	0.45	0/189	0.65	0/259

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	BF	0.45	0/189	0.63	0/259
2	BG	0.43	0/189	0.63	0/259
2	BH	0.45	0/189	0.63	0/259
2	BI	0.44	0/189	0.64	0/259
2	BJ	0.49	0/189	0.64	0/259
2	BK	0.46	0/189	0.64	0/259
2	BL	0.46	0/189	0.65	0/259
2	BM	0.46	0/189	0.64	0/259
2	BN	0.41	0/189	0.64	0/259
2	BO	0.43	0/189	0.64	0/259
2	BP	0.46	0/189	0.63	0/259
2	BQ	0.44	0/189	0.64	0/259
2	BR	0.45	0/189	0.65	0/259
2	BS	0.44	0/189	0.63	0/259
2	BT	0.45	0/189	0.64	0/259
2	BU	0.45	0/189	0.64	0/259
2	BV	0.46	0/189	0.65	0/259
2	BW	0.45	0/189	0.65	0/259
2	BX	0.45	0/189	0.64	0/259
2	BY	0.49	0/189	0.66	0/259
2	BZ	0.43	0/189	0.63	0/259
2	Ba	0.43	0/189	0.63	0/259
2	Bb	0.47	0/189	0.65	0/259
2	Bc	0.43	0/189	0.64	0/259
2	Bd	0.46	0/189	0.65	0/259
2	Be	0.44	0/189	0.64	0/259
2	Bf	0.46	0/189	0.64	0/259
2	Bg	0.68	1/189 (0.5%)	0.67	0/259
2	Bh	0.44	0/189	0.64	0/259
2	Bi	0.45	0/189	0.63	0/259
2	Bj	0.46	0/189	0.63	0/259
2	Bk	0.45	0/189	0.64	0/259
2	Bl	0.44	0/189	0.63	0/259
2	Bm	0.46	0/189	0.63	0/259
2	Bn	0.43	0/189	0.64	0/259
2	Bo	0.47	0/189	0.65	0/259
2	Bp	0.49	0/189	0.65	0/259
2	Bq	0.45	0/189	0.64	0/259
2	Br	0.45	0/189	0.64	0/259
2	Bs	0.49	0/189	0.65	0/259
2	Bt	0.46	0/189	0.63	0/259
2	Bu	0.43	0/189	0.64	0/259
2	Bv	0.44	0/189	0.64	0/259

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Bw	0.45	0/189	0.63	0/259
2	Bx	0.47	0/189	0.65	0/259
All	All	0.52	1/81240 (0.0%)	0.64	0/109980

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Bg	21	PRO	CA-CB	-5.07	1.43	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A0	1143	0	1145	37	0
1	A1	1143	0	1145	36	0
1	A2	1143	0	1145	35	0
1	A3	1143	0	1145	36	0
1	A4	1143	0	1145	35	0
1	A5	1143	0	1145	37	0
1	A6	1143	0	1145	37	0
1	A7	1143	0	1145	37	0
1	A8	1143	0	1145	32	0
1	A9	1143	0	1145	34	0
1	AA	1143	0	1145	39	0
1	AB	1143	0	1145	39	0
1	AC	1143	0	1145	41	0
1	AD	1143	0	1145	38	0
1	AE	1143	0	1145	38	0
1	AF	1143	0	1145	37	0
1	AG	1143	0	1145	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AH	1143	0	1145	40	0
1	AI	1143	0	1145	39	0
1	AJ	1143	0	1145	35	0
1	AK	1143	0	1145	39	0
1	AL	1143	0	1145	38	0
1	AM	1143	0	1145	41	0
1	AN	1143	0	1145	37	0
1	AO	1143	0	1145	39	0
1	AP	1143	0	1145	34	0
1	AQ	1143	0	1145	38	0
1	AR	1143	0	1145	37	0
1	AS	1143	0	1145	45	0
1	AT	1143	0	1145	45	0
1	AU	1143	0	1145	44	0
1	AV	1143	0	1145	52	0
1	AW	1143	0	1145	46	0
1	AX	1143	0	1145	48	0
1	AY	1143	0	1145	34	0
1	AZ	1143	0	1145	33	0
1	Aa	1143	0	1145	0	0
1	Ab	1143	0	1145	0	0
1	Ac	1143	0	1145	0	0
1	Ad	1143	0	1145	0	0
1	Ae	1143	0	1145	0	0
1	Af	1143	0	1145	0	0
1	Ag	1143	0	1145	0	0
1	Ah	1143	0	1145	0	0
1	Ai	1143	0	1145	0	0
1	Aj	1143	0	1145	0	0
1	Ak	1143	0	1145	0	0
1	Al	1143	0	1145	0	0
1	Am	1143	0	1145	0	0
1	An	1143	0	1145	0	0
1	Ao	1143	0	1145	0	0
1	Ap	1143	0	1145	0	0
1	Aq	1143	0	1145	0	0
1	Ar	1143	0	1145	0	0
1	As	1143	0	1145	0	0
1	At	1143	0	1145	0	0
1	Au	1143	0	1145	0	0
1	Av	1143	0	1145	0	0
1	Aw	1143	0	1145	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ax	1143	0	1145	0	0
2	B0	185	0	186	4	0
2	B1	185	0	186	10	0
2	B2	185	0	186	4	0
2	B3	185	0	186	6	1
2	B4	185	0	186	8	0
2	B5	185	0	186	4	1
2	B6	185	0	186	4	0
2	B7	185	0	186	5	0
2	B8	185	0	186	3	0
2	B9	185	0	186	5	0
2	BA	185	0	186	4	0
2	BB	185	0	186	4	0
2	BC	185	0	186	4	0
2	BD	185	0	186	8	0
2	BE	185	0	186	4	0
2	BF	185	0	186	4	0
2	BG	185	0	186	16	0
2	BH	185	0	186	9	0
2	BI	185	0	186	5	0
2	BJ	185	0	186	4	0
2	BK	185	0	186	4	0
2	BL	185	0	186	5	0
2	BM	185	0	186	4	0
2	BN	185	0	186	4	0
2	BO	185	0	186	5	0
2	BP	185	0	186	10	0
2	BQ	185	0	186	5	0
2	BR	185	0	186	4	0
2	BS	185	0	186	6	0
2	BT	185	0	186	5	0
2	BU	185	0	186	5	0
2	BV	185	0	186	18	0
2	BW	185	0	186	4	0
2	BX	185	0	186	11	0
2	BY	185	0	186	4	4
2	BZ	185	0	186	5	0
2	Ba	185	0	186	0	0
2	Bb	185	0	186	0	0
2	Bc	185	0	186	0	0
2	Bd	185	0	186	0	0
2	Be	185	0	186	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Bf	185	0	186	0	0
2	Bg	185	0	186	0	4
2	Bh	185	0	186	0	0
2	Bi	185	0	186	0	0
2	Bj	185	0	186	0	0
2	Bk	185	0	186	0	0
2	Bl	185	0	186	0	0
2	Bm	185	0	186	0	0
2	Bn	185	0	186	0	0
2	Bo	185	0	186	0	0
2	Bp	185	0	186	0	0
2	Bq	185	0	186	0	0
2	Br	185	0	186	0	0
2	Bs	185	0	186	0	0
2	Bt	185	0	186	0	0
2	Bu	185	0	186	0	0
2	Bv	185	0	186	0	0
2	Bw	185	0	186	0	0
2	Bx	185	0	186	0	0
3	A1	1	0	0	0	0
3	A4	2	0	0	0	0
3	A5	2	0	0	0	0
3	A6	2	0	0	0	0
3	A7	1	0	0	0	0
3	A8	2	0	0	0	0
3	A9	2	0	0	0	0
3	AA	2	0	0	0	0
3	AB	1	0	0	0	0
3	AC	1	0	0	0	0
3	AD	1	0	0	0	0
3	AF	1	0	0	0	0
3	AJ	1	0	0	0	0
3	AN	1	0	0	0	0
3	AO	1	0	0	0	0
3	AQ	2	0	0	0	0
3	AR	1	0	0	0	0
3	Aa	1	0	0	0	0
3	Ac	2	0	0	0	0
3	Ad	1	0	0	0	0
3	Af	1	0	0	0	0
3	Ah	1	0	0	0	0
3	Ak	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Am	1	0	0	0	0
3	An	1	0	0	0	0
3	Ap	1	0	0	0	0
3	Aq	1	0	0	0	0
3	Ar	1	0	0	0	0
3	As	1	0	0	0	0
3	Av	1	0	0	0	0
3	Aw	2	0	0	0	0
All	All	79720	0	79860	1332	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 1332 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AE:242:ASN:H	1:AQ:235:ASN:HD21	1.01	1.03
1:AL:235:ASN:HD21	1:AR:242:ASN:H	1.06	1.01
1:AA:242:ASN:H	1:AM:235:ASN:HD21	1.06	1.00
1:AS:235:ASN:HD21	1:AU:242:ASN:H	99.01	0.99
1:AJ:235:ASN:HD21	1:AP:242:ASN:H	1.07	0.99

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:BY:18:PRO:O	2:Bg:21:PRO:CB[2.655]	1.60	0.60
2:B3:23:GLU:OE2	2:B5:20:VAL:CG1[2.546]	1.87	0.33
2:BY:19:CYS:CA	2:Bg:21:PRO:CG[2.655]	1.91	0.29
2:BY:18:PRO:C	2:Bg:21:PRO:CB[2.655]	2.01	0.19
2:BY:20:VAL:CA	2:Bg:19:CYS:O[2.655]	2.16	0.04

## 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	A0	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A1	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A2	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A3	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A4	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	A5	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A6	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	A7	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	A8	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	A9	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AA	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AB	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	AC	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AD	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	AE	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	AF	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AG	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AH	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AI	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AJ	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AK	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	AL	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AM	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AN	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AO	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AP	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AQ	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AR	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	AS	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AT	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	AU	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AV	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AW	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AX	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	AY	142/148 (96%)	134 (94%)	7 (5%)	1 (1%)	30	81
1	AZ	142/148 (96%)	134 (94%)	7 (5%)	1 (1%)	30	81
1	Aa	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Ab	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Ac	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Ad	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Ae	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Af	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Ag	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Ah	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Ai	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Aj	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Ak	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Al	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	Am	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	An	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	Ao	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	Ap	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Aq	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	30	81
1	Ar	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	As	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	At	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Au	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Av	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
1	Aw	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	30	81
1	Ax	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	30	81
2	B0	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B1	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B2	23/63 (36%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B3	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B4	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B5	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B6	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B7	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B8	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	B9	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BA	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BB	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BC	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BD	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BE	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BF	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BG	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BH	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BI	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BJ	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BK	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BL	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BM	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BN	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BO	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BP	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BQ	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BR	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BS	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BT	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BU	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BV	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BW	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	BX	23/63 (36%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BY	23/63 (36%)	21 (91%)	2 (9%)	0	100	100
2	BZ	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Ba	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bb	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bc	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bd	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Be	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bf	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bg	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bh	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bi	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bj	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bk	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bl	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bm	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bn	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bo	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bp	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bq	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Br	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bs	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bt	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bu	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bv	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bw	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
2	Bx	23/63 (36%)	22 (96%)	1 (4%)	0	100	100
All	All	9900/12660 (78%)	9474 (96%)	366 (4%)	60 (1%)	33	83

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	161	GLY
1	AB	161	GLY

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Mol	Chain	Res	Type
1	AC	161	GLY
1	AD	161	GLY
1	AE	161	GLY

### 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	A0	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	A1	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	A2	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A3	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	A4	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A5	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A6	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A7	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A8	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	A9	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AA	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AB	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AC	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AD	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AE	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	AF	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	AG	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AH	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AI	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AJ	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AK	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AL	126/130 (97%)	120 (95%)	6 (5%)	35	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AM	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	AN	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AO	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AP	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AQ	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AR	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AS	126/130 (97%)	122 (97%)	4 (3%)	51	88
1	AT	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	AU	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AV	126/130 (97%)	119 (94%)	7 (6%)	30	75
1	AW	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AX	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	AY	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	AZ	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Aa	126/130 (97%)	122 (97%)	4 (3%)	51	88
1	Ab	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Ac	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ad	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ae	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Af	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ag	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ah	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ai	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Aj	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ak	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Al	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Am	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	An	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Ao	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Ap	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Aq	126/130 (97%)	120 (95%)	6 (5%)	35	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ar	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	As	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	At	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Au	126/130 (97%)	121 (96%)	5 (4%)	42	83
1	Av	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Aw	126/130 (97%)	120 (95%)	6 (5%)	35	79
1	Ax	126/130 (97%)	120 (95%)	6 (5%)	35	79
2	B0	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B1	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B2	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B3	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B4	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B5	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B6	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B7	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B8	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	B9	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BA	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BB	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BC	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BD	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BE	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BF	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BG	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BH	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BI	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BJ	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BK	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BL	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BM	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BN	22/51 (43%)	21 (96%)	1 (4%)	38	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BO	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BP	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BQ	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BR	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BS	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BT	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BU	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BV	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BW	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BX	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BY	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	BZ	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Ba	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bb	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bc	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bd	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Be	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bf	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bg	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bh	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bi	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bj	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bk	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bl	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bm	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bn	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bo	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bp	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bq	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Br	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bs	22/51 (43%)	21 (96%)	1 (4%)	38	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bt	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bu	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bv	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bw	22/51 (43%)	21 (96%)	1 (4%)	38	81
2	Bx	22/51 (43%)	21 (96%)	1 (4%)	38	81
All	All	8880/10860 (82%)	8500 (96%)	380 (4%)	40	82

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A6	233	ILE
1	Ae	239	THR
2	B5	31	HIS
1	A7	233	ILE
1	Aa	239	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 183 such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	210	HIS
1	A7	235	ASN
1	At	218	HIS
1	A2	210	HIS
1	A4	218	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 40 ligands modelled in this entry, 40 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<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	A0	144/148 (97%)	-0.32	0 100 100	19, 36, 57, 67	0
1	A1	144/148 (97%)	-0.27	0 100 100	18, 36, 58, 67	0
1	A2	144/148 (97%)	-0.30	0 100 100	19, 36, 58, 67	0
1	A3	144/148 (97%)	-0.25	0 100 100	18, 35, 57, 66	0
1	A4	144/148 (97%)	-0.17	0 100 100	21, 38, 60, 68	0
1	A5	144/148 (97%)	-0.27	0 100 100	18, 35, 57, 65	0
1	A6	144/148 (97%)	-0.32	0 100 100	19, 37, 59, 67	0
1	A7	144/148 (97%)	-0.28	0 100 100	18, 36, 57, 66	0
1	A8	144/148 (97%)	-0.33	0 100 100	18, 37, 59, 66	0
1	A9	144/148 (97%)	-0.29	0 100 100	16, 35, 57, 66	0
1	AA	144/148 (97%)	-0.20	0 100 100	23, 38, 60, 68	0
1	AB	144/148 (97%)	-0.29	0 100 100	18, 37, 59, 66	0
1	AC	144/148 (97%)	-0.27	0 100 100	20, 38, 59, 68	0
1	AD	144/148 (97%)	-0.26	0 100 100	15, 34, 57, 65	0
1	AE	144/148 (97%)	-0.31	0 100 100	21, 37, 59, 68	0
1	AF	144/148 (97%)	-0.30	0 100 100	18, 36, 57, 67	0
1	AG	144/148 (97%)	-0.20	0 100 100	21, 38, 59, 68	0
1	AH	144/148 (97%)	-0.28	0 100 100	19, 36, 58, 67	0
1	AI	144/148 (97%)	-0.26	0 100 100	20, 38, 59, 68	0
1	AJ	144/148 (97%)	-0.27	0 100 100	17, 34, 57, 66	0
1	AK	144/148 (97%)	-0.33	0 100 100	20, 37, 58, 67	0
1	AL	144/148 (97%)	-0.28	0 100 100	17, 34, 57, 66	0
1	AM	144/148 (97%)	-0.26	0 100 100	22, 39, 59, 68	0
1	AN	144/148 (97%)	-0.30	0 100 100	18, 36, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	AO	144/148 (97%)	-0.30	0	100	100	20, 38, 60, 68	0
1	AP	144/148 (97%)	-0.27	0	100	100	15, 35, 58, 67	0
1	AQ	144/148 (97%)	-0.34	0	100	100	20, 37, 58, 66	0
1	AR	144/148 (97%)	-0.28	0	100	100	18, 36, 58, 67	0
1	AS	144/148 (97%)	-0.23	0	100	100	21, 38, 59, 68	0
1	AT	144/148 (97%)	-0.29	0	100	100	18, 36, 57, 66	0
1	AU	144/148 (97%)	-0.32	0	100	100	20, 36, 58, 67	0
1	AV	144/148 (97%)	-0.31	0	100	100	17, 36, 58, 66	0
1	AW	144/148 (97%)	-0.30	0	100	100	20, 37, 58, 67	0
1	AX	144/148 (97%)	-0.29	0	100	100	16, 35, 58, 66	0
1	AY	144/148 (97%)	-0.20	0	100	100	22, 38, 59, 68	0
1	AZ	144/148 (97%)	-0.28	0	100	100	19, 36, 57, 66	0
1	Aa	144/148 (97%)	-0.29	0	100	100	19, 38, 59, 67	0
1	Ab	144/148 (97%)	-0.31	0	100	100	17, 35, 57, 66	0
1	Ac	144/148 (97%)	-0.33	0	100	100	21, 38, 59, 68	0
1	Ad	144/148 (97%)	-0.29	0	100	100	16, 34, 57, 66	0
1	Ae	144/148 (97%)	-0.30	0	100	100	20, 37, 59, 67	0
1	Af	144/148 (97%)	-0.28	0	100	100	20, 37, 59, 67	0
1	Ag	144/148 (97%)	-0.28	0	100	100	20, 37, 58, 67	0
1	Ah	144/148 (97%)	-0.27	0	100	100	18, 35, 57, 66	0
1	Ai	144/148 (97%)	-0.28	0	100	100	21, 38, 59, 68	0
1	Aj	144/148 (97%)	-0.28	0	100	100	17, 35, 57, 66	0
1	Ak	144/148 (97%)	-0.31	0	100	100	19, 37, 59, 67	0
1	Al	144/148 (97%)	-0.32	0	100	100	20, 37, 59, 68	0
1	Am	144/148 (97%)	-0.28	0	100	100	19, 36, 58, 68	0
1	An	144/148 (97%)	-0.27	0	100	100	17, 35, 58, 66	0
1	Ao	144/148 (97%)	-0.30	0	100	100	21, 38, 59, 68	0
1	Ap	144/148 (97%)	-0.30	0	100	100	16, 35, 58, 66	0
1	Aq	144/148 (97%)	-0.30	0	100	100	19, 37, 59, 68	0
1	Ar	144/148 (97%)	-0.29	1 (0%)	84	42	19, 37, 58, 67	0
1	As	144/148 (97%)	-0.31	0	100	100	18, 36, 58, 66	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	At	144/148 (97%)	-0.27	0	100	100	18, 35, 57, 66	0
1	Au	144/148 (97%)	-0.30	0	100	100	20, 36, 58, 68	0
1	Av	144/148 (97%)	-0.27	0	100	100	19, 37, 58, 67	0
1	Aw	144/148 (97%)	-0.29	0	100	100	18, 36, 58, 66	0
1	Ax	144/148 (97%)	-0.26	0	100	100	17, 35, 57, 66	0
2	B0	25/63 (39%)	0.53	2 (8%)	12	4	55, 91, 126, 136	0
2	B1	25/63 (39%)	0.66	4 (16%)	3	1	56, 92, 126, 136	0
2	B2	25/63 (39%)	0.64	2 (8%)	12	4	55, 91, 126, 135	0
2	B3	25/63 (39%)	0.60	2 (8%)	12	4	55, 90, 125, 135	0
2	B4	25/63 (39%)	0.83	2 (8%)	12	4	58, 93, 126, 136	0
2	B5	25/63 (39%)	0.73	3 (12%)	5	2	55, 90, 125, 136	0
2	B6	25/63 (39%)	0.50	3 (12%)	5	2	57, 91, 126, 136	0
2	B7	25/63 (39%)	0.69	3 (12%)	5	2	55, 91, 126, 136	0
2	B8	25/63 (39%)	0.73	3 (12%)	5	2	55, 91, 126, 136	0
2	B9	25/63 (39%)	0.65	3 (12%)	5	2	55, 91, 125, 135	0
2	BA	25/63 (39%)	0.79	3 (12%)	5	2	58, 92, 126, 136	0
2	BB	25/63 (39%)	0.58	3 (12%)	5	2	57, 92, 126, 136	0
2	BC	25/63 (39%)	0.75	1 (4%)	36	8	57, 92, 126, 135	0
2	BD	25/63 (39%)	0.89	3 (12%)	5	2	54, 89, 125, 136	0
2	BE	25/63 (39%)	0.69	4 (16%)	3	1	57, 92, 126, 136	0
2	BF	25/63 (39%)	0.70	4 (16%)	3	1	56, 91, 126, 135	0
2	BG	25/63 (39%)	0.94	5 (20%)	2	1	57, 93, 126, 135	0
2	BH	25/63 (39%)	0.66	2 (8%)	12	4	55, 90, 126, 136	0
2	BI	25/63 (39%)	0.69	2 (8%)	12	4	57, 92, 126, 135	0
2	BJ	25/63 (39%)	0.61	2 (8%)	12	4	54, 91, 125, 135	0
2	BK	25/63 (39%)	0.76	3 (12%)	5	2	57, 92, 126, 135	0
2	BL	25/63 (39%)	0.68	3 (12%)	5	2	54, 89, 125, 135	0
2	BM	25/63 (39%)	0.96	5 (20%)	2	1	58, 93, 126, 136	0
2	BN	25/63 (39%)	0.69	5 (20%)	2	1	55, 92, 125, 135	0
2	BO	25/63 (39%)	0.75	3 (12%)	5	2	58, 93, 126, 136	0
2	BP	25/63 (39%)	0.67	3 (12%)	5	2	54, 90, 126, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
2	BQ	25/63 (39%)	0.67	3 (12%)	5	2	56, 91, 126, 136	0
2	BR	25/63 (39%)	0.69	2 (8%)	12	4	55, 92, 125, 136	0
2	BS	25/63 (39%)	0.72	3 (12%)	5	2	57, 93, 126, 136	0
2	BT	25/63 (39%)	0.76	4 (16%)	3	1	56, 92, 126, 136	0
2	BU	25/63 (39%)	0.66	2 (8%)	12	4	56, 92, 126, 136	0
2	BV	25/63 (39%)	0.64	2 (8%)	12	4	56, 91, 126, 136	0
2	BW	25/63 (39%)	0.65	2 (8%)	12	4	57, 92, 126, 136	0
2	BX	25/63 (39%)	0.66	3 (12%)	5	2	55, 91, 126, 136	0
2	BY	25/63 (39%)	0.95	4 (16%)	3	1	58, 92, 126, 136	0
2	BZ	25/63 (39%)	0.63	3 (12%)	5	2	54, 90, 125, 136	0
2	Ba	25/63 (39%)	0.69	2 (8%)	12	4	56, 91, 126, 136	0
2	Bb	25/63 (39%)	0.65	2 (8%)	12	4	54, 90, 125, 135	0
2	Bc	25/63 (39%)	0.73	4 (16%)	3	1	57, 92, 125, 135	0
2	Bd	25/63 (39%)	0.57	2 (8%)	12	4	54, 91, 125, 136	0
2	Be	25/63 (39%)	0.71	4 (16%)	3	1	56, 91, 126, 136	0
2	Bf	25/63 (39%)	1.01	3 (12%)	5	2	58, 92, 126, 136	0
2	Bg	25/63 (39%)	1.18	6 (24%)	1	1	56, 92, 126, 135	0
2	Bh	25/63 (39%)	0.67	4 (16%)	3	1	54, 91, 126, 135	0
2	Bi	25/63 (39%)	0.78	2 (8%)	12	4	57, 92, 126, 136	0
2	Bj	25/63 (39%)	0.73	3 (12%)	5	2	54, 90, 125, 136	0
2	Bk	25/63 (39%)	0.65	3 (12%)	5	2	56, 91, 125, 136	0
2	Bl	25/63 (39%)	0.69	3 (12%)	5	2	56, 92, 125, 135	0
2	Bm	25/63 (39%)	0.65	4 (16%)	3	1	56, 92, 126, 136	0
2	Bn	25/63 (39%)	0.54	2 (8%)	12	4	55, 91, 126, 136	0
2	Bo	25/63 (39%)	0.58	4 (16%)	3	1	57, 91, 126, 136	0
2	Bp	25/63 (39%)	0.87	3 (12%)	5	2	54, 89, 125, 136	0
2	Bq	25/63 (39%)	0.84	5 (20%)	2	1	56, 92, 126, 136	0
2	Br	25/63 (39%)	0.77	3 (12%)	5	2	57, 92, 126, 135	0
2	Bs	25/63 (39%)	0.56	3 (12%)	5	2	55, 90, 125, 136	0
2	Bt	25/63 (39%)	0.66	2 (8%)	12	4	54, 91, 125, 136	0
2	Bu	25/63 (39%)	0.60	2 (8%)	12	4	56, 92, 126, 136	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
2	Bv	25/63 (39%)	0.48	3 (12%) 5 2	55, 91, 125, 136	0
2	Bw	25/63 (39%)	0.73	3 (12%) 5 2	55, 91, 125, 136	0
2	Bx	25/63 (39%)	0.68	3 (12%) 5 2	54, 89, 126, 135	0
All	All	10140/12660 (80%)	-0.14	182 (1%) 65 20	15, 39, 106, 136	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Bf	41	PRO	6.5
2	BR	41	PRO	6.0
2	B7	41	PRO	5.7
2	Bp	41	PRO	5.7
2	B5	41	PRO	5.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	AN	301	1/1	1.37	92.53	69,69,69,69	0
3	MG	AJ	301	1/1	1.11	88.70	46,46,46,46	0
3	MG	Ac	302	1/1	1.86	86.52	68,68,68,68	0
3	MG	Aw	302	1/1	0.90	78.40	38,38,38,38	0
3	MG	An	301	1/1	1.02	76.98	41,41,41,41	0
3	MG	AO	301	1/1	1.39	73.04	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	Aq	301	1/1	0.96	55.53	45,45,45,45	0
3	MG	A9	302	1/1	1.11	53.63	62,62,62,62	0
3	MG	A5	302	1/1	1.06	45.09	36,36,36,36	0
3	MG	AR	301	1/1	1.05	44.97	59,59,59,59	0
3	MG	AQ	302	1/1	1.01	43.45	59,59,59,59	0
3	MG	Ar	301	1/1	1.13	42.73	61,61,61,61	0
3	MG	A6	302	1/1	0.98	40.95	45,45,45,45	0
3	MG	AA	1002	1/1	1.50	40.35	63,63,63,63	0
3	MG	A7	301	1/1	1.15	36.68	42,42,42,42	0
3	MG	AD	301	1/1	0.44	32.37	25,25,25,25	0
3	MG	A8	302	1/1	1.32	32.09	54,54,54,54	0
3	MG	Av	301	1/1	0.81	31.17	35,35,35,35	0
3	MG	Am	301	1/1	0.98	31.12	49,49,49,49	0
3	MG	Ah	301	1/1	0.54	30.87	41,41,41,41	0
3	MG	AC	301	1/1	0.71	30.87	46,46,46,46	0
3	MG	Ap	301	1/1	0.76	30.25	32,32,32,32	0
3	MG	A4	302	1/1	1.00	30.24	73,73,73,73	0
3	MG	Ak	301	1/1	0.58	28.97	37,37,37,37	0
3	MG	AQ	301	1/1	0.73	21.90	25,25,25,25	0
3	MG	AB	301	1/1	0.38	20.03	35,35,35,35	0
3	MG	Ac	301	1/1	0.54	17.59	43,43,43,43	0
3	MG	A9	301	1/1	0.43	16.74	37,37,37,37	0
3	MG	AF	301	1/1	0.46	14.60	28,28,28,28	0
3	MG	A6	301	1/1	0.41	14.23	53,53,53,53	0
3	MG	Aw	301	1/1	0.30	9.98	20,20,20,20	0
3	MG	A8	301	1/1	0.50	8.65	22,22,22,22	0
3	MG	A1	301	1/1	0.41	8.63	20,20,20,20	0
3	MG	Ad	301	1/1	0.35	8.15	17,17,17,17	0
3	MG	A5	301	1/1	0.36	8.08	11,11,11,11	0
3	MG	As	301	1/1	0.29	7.57	21,21,21,21	0
3	MG	A4	301	1/1	0.35	5.75	44,44,44,44	0
3	MG	AA	1001	1/1	0.34	4.35	46,46,46,46	0
3	MG	Af	301	1/1	0.24	4.07	23,23,23,23	0
3	MG	Aa	301	1/1	0.26	3.65	28,28,28,28	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.