



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:30 PM GMT

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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

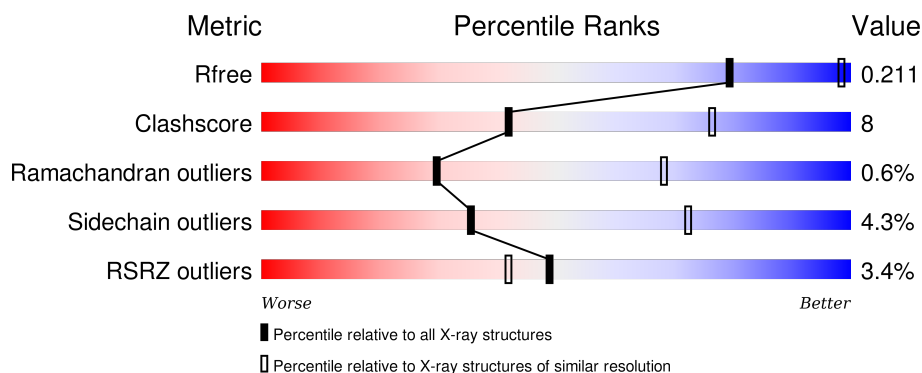
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.
















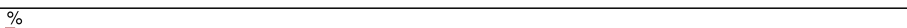











Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A0	148	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	A1	148	<div> <div>73%</div> <div>21%</div> <div>• •</div> </div>
1	A2	148	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	A3	148	<div> <div>2%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
1	A4	148	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>• •</div> </div>







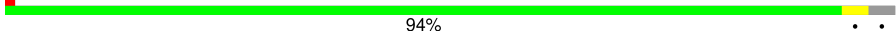






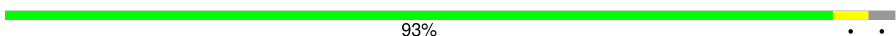

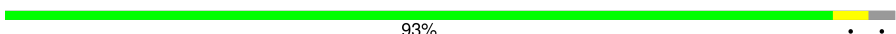
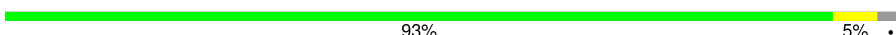
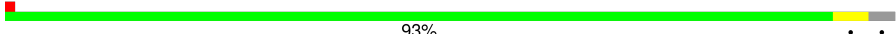
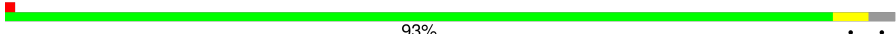




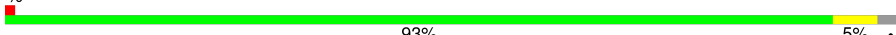

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Mol	Chain	Length	Quality of chain
1	A5	148	 71%24% . .
1	A6	148	 72%23% . .
1	A7	148	 72%23% . .
1	A8	148	 74%21% . .
1	A9	148	 73%22% . .
1	AA	148	 2%70%25% . .
1	AB	148	 70%24% . .
1	AC	148	 %69%26% . .
1	AD	148	 72%23% . .
1	AE	148	 %70%24% . .
1	AF	148	 72%22% . .
1	AG	148	 %71%24% . .
1	AH	148	 %70%25% . .
1	AI	148	 %70%25% . .
1	AJ	148	 73%22% . .
1	AK	148	 70%25% . .
1	AL	148	 70%24% . .
1	AM	148	 %68%26% . .
1	AN	148	 72%23% . .
1	AO	148	 70%24% . .
1	AP	148	 73%22% . .
1	AQ	148	 70%24% . .
1	AR	148	 72%22% . .
1	AS	148	 %73%22% . .
1	AT	148	 73%21% . .

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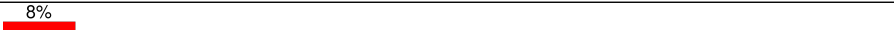

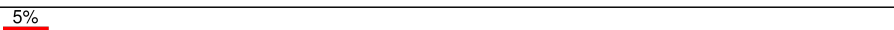
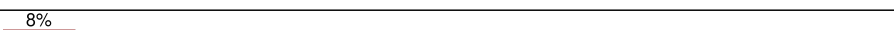











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Mol	Chain	Length	Quality of chain
1	AU	148	
1	AV	148	
1	AW	148	
1	AX	148	
1	AY	148	
1	AZ	148	
1	Aa	148	
1	Ab	148	
1	Ac	148	
1	Ad	148	
1	Ae	148	
1	Af	148	
1	Ag	148	
1	Ah	148	
1	Ai	148	
1	Aj	148	
1	Ak	148	
1	Al	148	
1	Am	148	
1	An	148	
1	Ao	148	
1	Ap	148	
1	Aq	148	
1	Ar	148	
1	As	148	

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Mol	Chain	Length	Quality of chain
1	At	148	 93% . .
1	Au	148	 93% . .
1	Av	148	 93% 5% .
1	Aw	148	 93% 5% .
1	Ax	148	 93% 5% .
2	B0	63	 5% 30% 10% 60%
2	B1	63	 8% 27% 13% 60%
2	B2	63	 10% 30% 10% 60%
2	B3	63	 5% 25% 14% 60%
2	B4	63	 14% 27% 13% 60%
2	B5	63	 8% 29% 11% 60%
2	B6	63	 6% 30% 10% 60%
2	B7	63	 5% 30% 10% 60%
2	B8	63	 8% 32% 8% 60%
2	B9	63	 8% 29% 11% 60%
2	BA	63	 11% 30% 10% 60%
2	BB	63	 8% 30% 10% 60%
2	BC	63	 13% 30% 10% 60%
2	BD	63	 8% 27% 13% 60%
2	BE	63	 11% 30% 10% 60%
2	BF	63	 8% 30% 10% 60%
2	BG	63	 14% 25% 14% 60%
2	BH	63	 8% 24% 16% 60%
2	BI	63	 8% 27% 13% 60%
2	BJ	63	 8% 30% 10% 60%

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Mol	Chain	Length	Quality of chain
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	
2	Bc	63	
2	Bd	63	
2	Be	63	
2	Bf	63	
2	Bg	63	
2	Bh	63	
2	Bi	63	

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Mol	Chain	Length	Quality of chain
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, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	AA	1001	-	-	-	X
3	MG	AA	1002	-	-	-	X
3	MG	AB	301	-	-	-	X
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 [i](#)

There are 3 unique types of molecules in this entry. The entry contains 79720 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 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

*Continued on next page...*

*Continued from previous page...*

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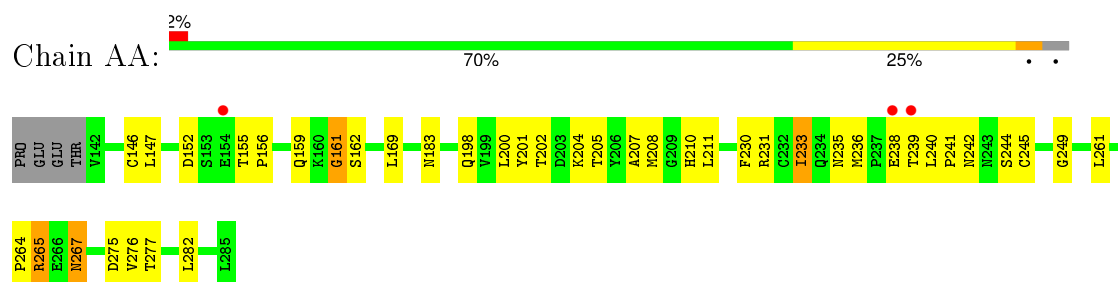
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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3	Aa	1	Total 1	Mg 1	0	0
3	A4	2	Total 2	Mg 2	0	0
3	Ar	1	Total 1	Mg 1	0	0
3	A9	2	Total 2	Mg 2	0	0
3	Am	1	Total 1	Mg 1	0	0
3	AQ	2	Total 2	Mg 2	0	0
3	Ad	1	Total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

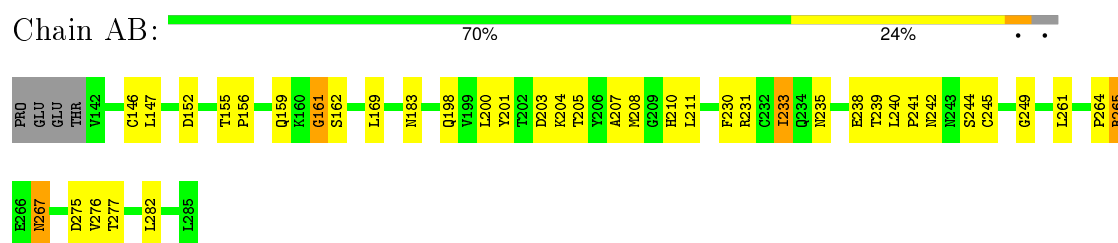
### 3 Residue-property plots [i](#)

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

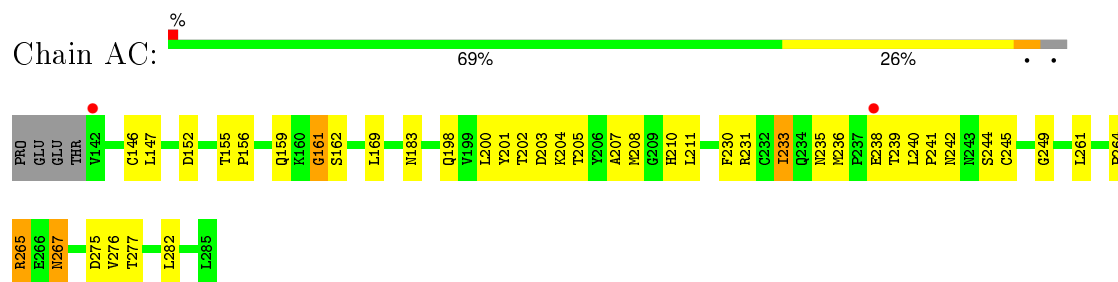
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



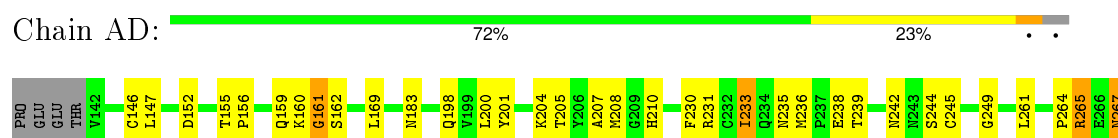
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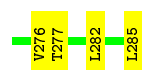


- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

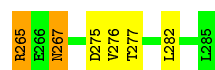


- Molecule 1: Tumor necrosis factor ligand superfamily member 13B





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



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



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



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



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





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

Chain AJ: 73% 22%



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

Chain AK: 70% 25%



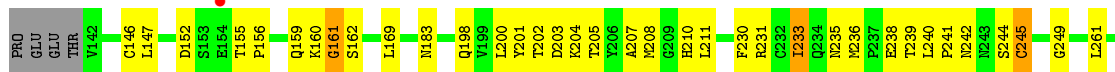
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AL: 70% 24%



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

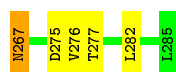
Chain AM: 68% 26%



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

Chain AN: 72% 23%





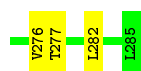
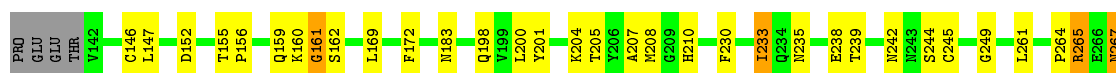
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AO: 70% 24%



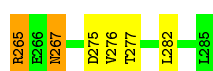
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AP: 73% 22%



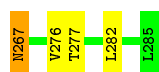
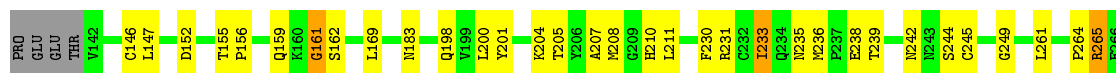
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AQ: 70% 24%



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

Chain AR: 72% 22%

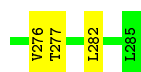


- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AS: 73% 22%

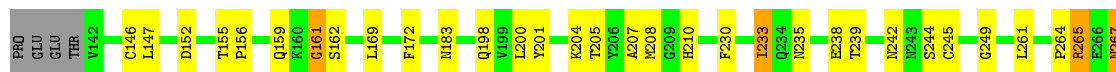






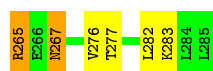
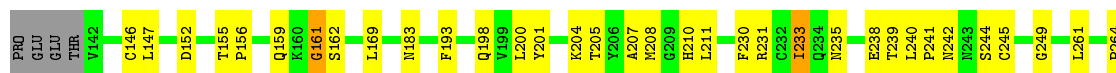
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AT: 73% 21% . .



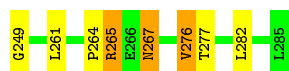
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AU: 70% 24% . .



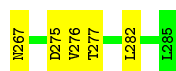
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AV: 68% 25% . .



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

Chain AW: 72% 23% . .



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

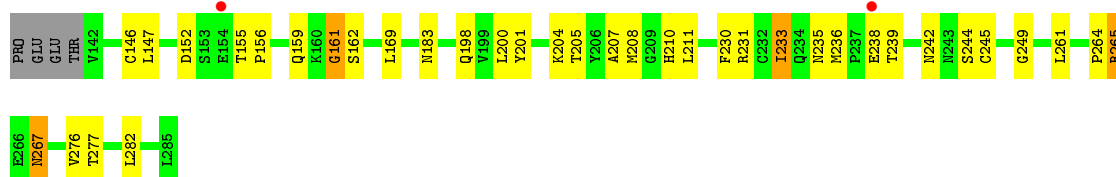
Chain AX: 69% 25% . .





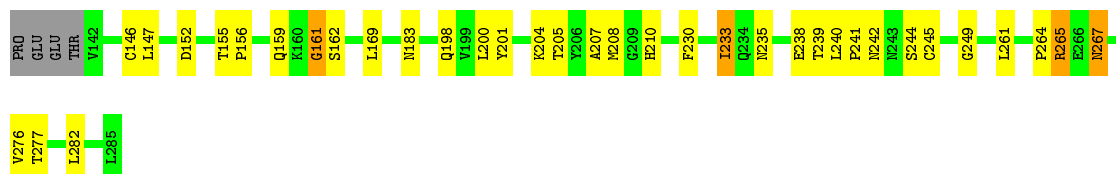
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AY: %



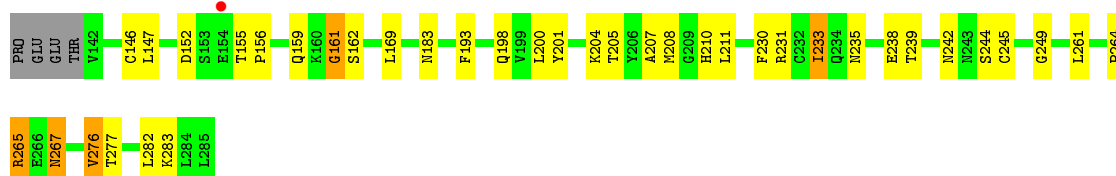
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain AZ: %



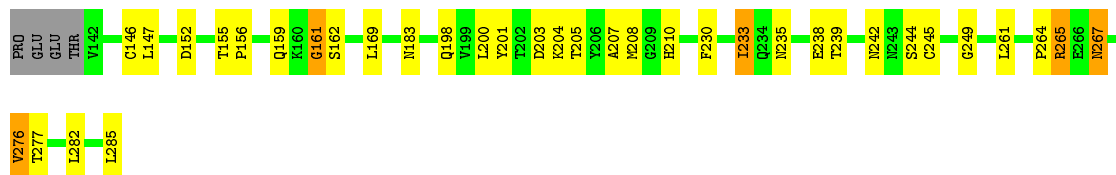
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A0: %



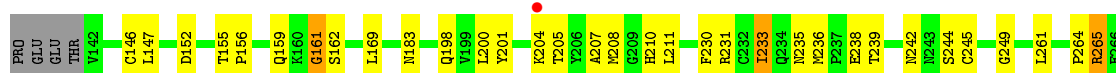
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

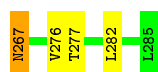
Chain A1: %



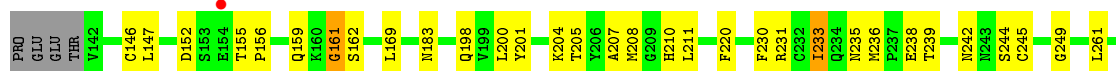
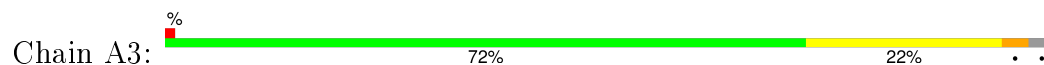
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A2: %

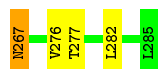
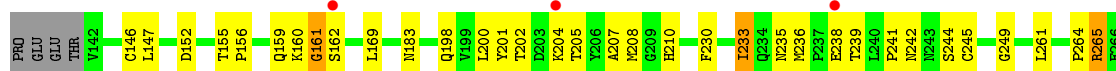
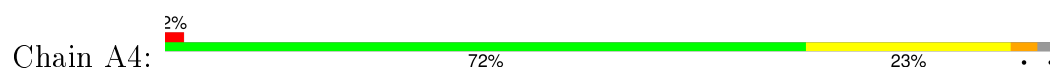




- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



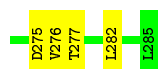
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



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



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



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





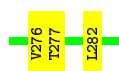
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain A8: 74% 21%



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

Chain A9: 73% 22%



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

Chain Aa: 94% 5%



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

Chain Ab: 93% 5%



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

Chain Ac: 93% 5%



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

Chain Ad: 93% 5%



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

Chain Ae:  93% 5% .



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

Chain Af:  93% . .



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

Chain Ag:  93% . .



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

Chain Ah:  93% . .



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

Chain Ai:  93% . .



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

Chain Aj:  93% . .



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

Chain Ak:  93% 5% .



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



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



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



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



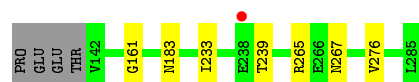
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B



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



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



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

Chain As:  93% 5% .



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

Chain At:  93% . .



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

Chain Au:  93% . .



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

Chain Av:  93% 5% .



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

Chain Aw:  93% 5% .




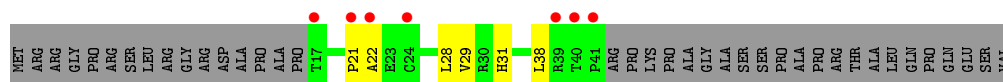
- Molecule 1: Tumor necrosis factor ligand superfamily member 13B

Chain Ax:  93% 5% .



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

Chain BA:  11% 30% 10% 60%

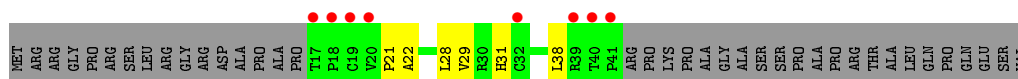
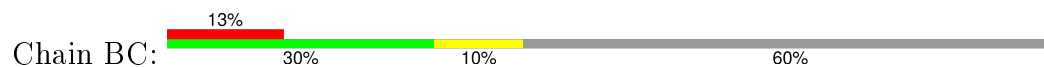


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

Chain BB:  8% 30% 10% 60%



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



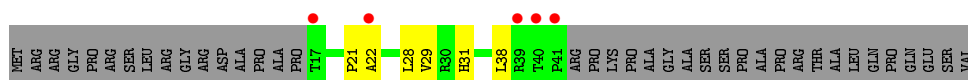
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



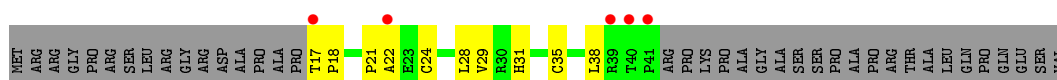
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



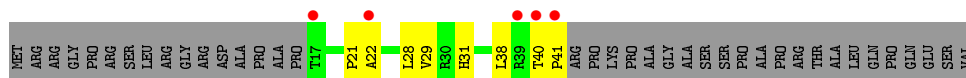
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



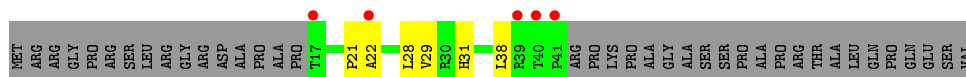
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



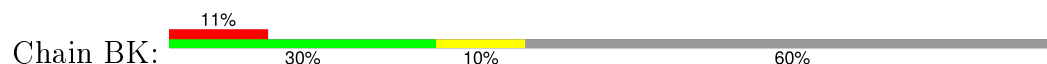




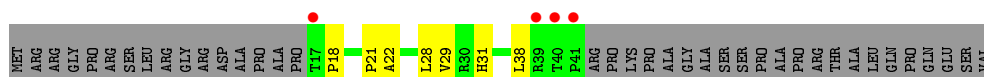
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



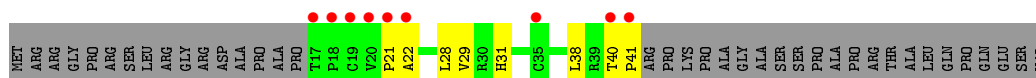
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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

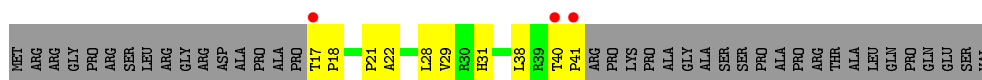


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

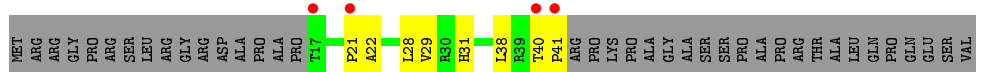


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C





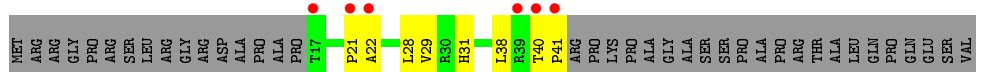
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



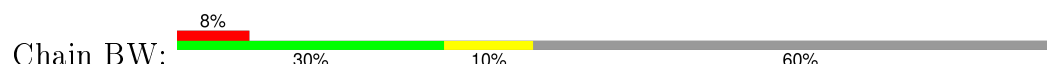
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

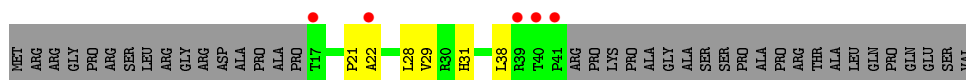


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

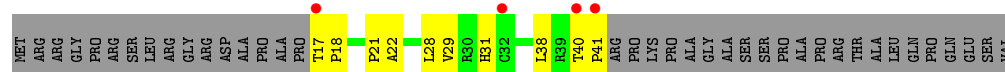


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

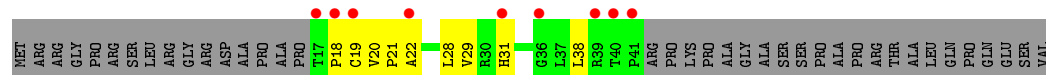




- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



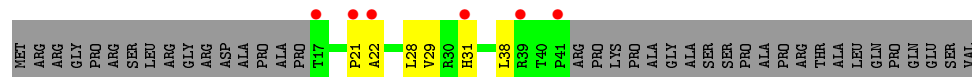
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



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



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

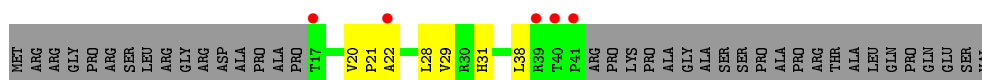




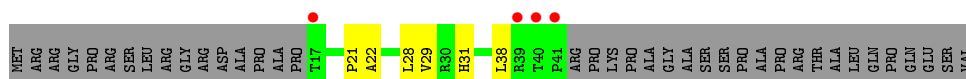
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



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



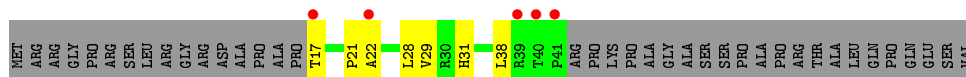
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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

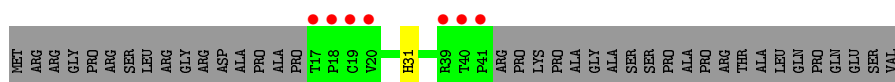


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

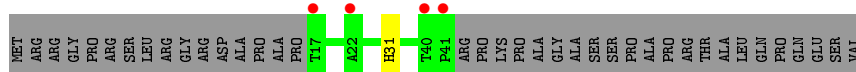


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C





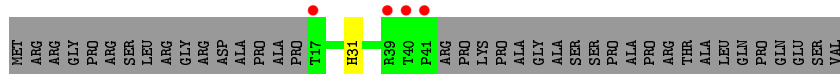
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



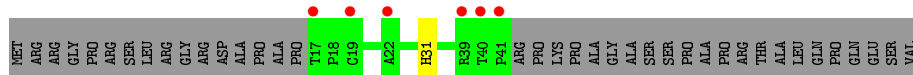
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



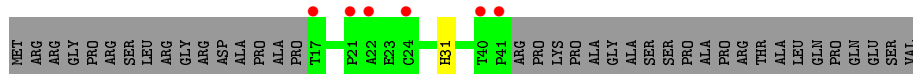
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



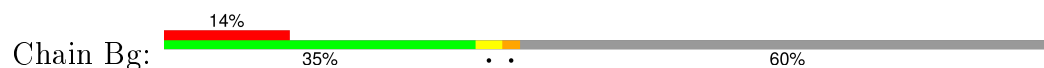
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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

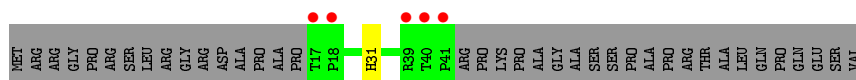


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

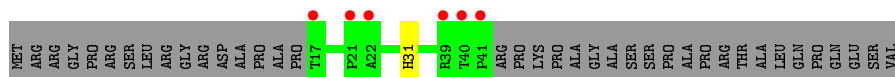


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

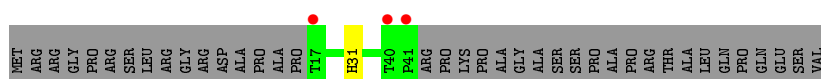




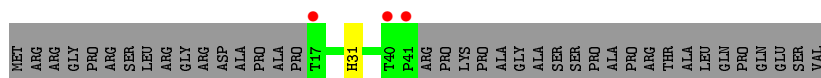
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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



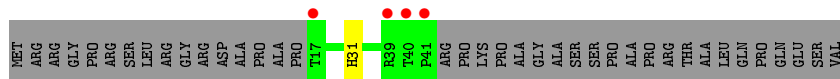
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



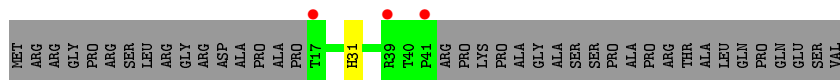
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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

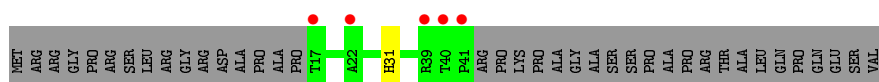


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

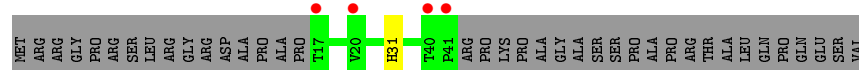


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

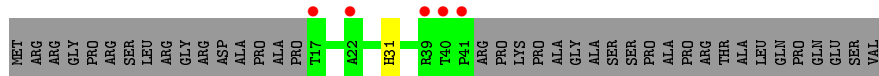




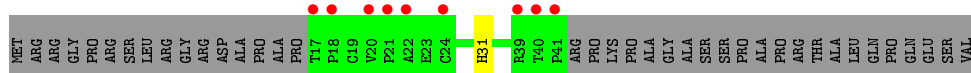
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



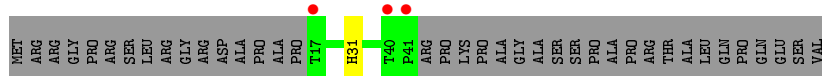
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



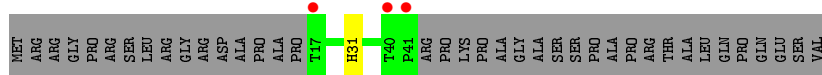
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



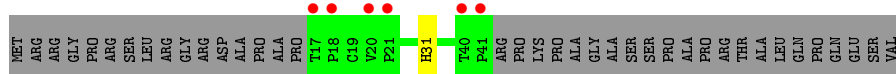
- Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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

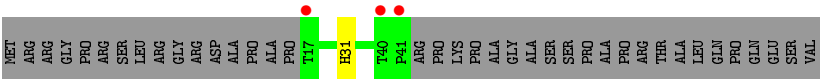


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

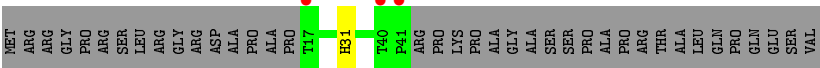


- Molecule 2: Tumor necrosis factor receptor superfamily member 13C

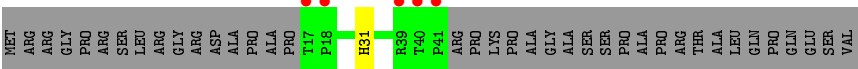




● Molecule 2: Tumor necrosis factor receptor superfamily member 13C



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





## 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 0.204 , 0.211	Depositor DCC
$R_{free}$ test set	13477 reflections (5.51%)	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 , 33.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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
1	AH	1143	0	1145	40	0
1	AI	1143	0	1145	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
1	Ax	1143	0	1145	0	0
2	B0	185	0	186	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
2	Bf	185	0	186	0	0
2	Bg	185	0	186	0	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	Am	1	0	0	0	0
3	An	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 8.

The worst 5 of 1332 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: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	Interatomic distance (Å)	Clash overlap (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 [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A0	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A1	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A2	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A3	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A4	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	A5	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A6	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	A7	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	A8	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	A9	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AA	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AB	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	AC	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AD	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	AE	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	AF	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AG	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AH	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AI	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AJ	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AK	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	AL	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AM	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AN	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AO	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AP	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AQ	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AR	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	AS	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AT	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	AU	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AV	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AW	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AX	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	AY	142/148 (96%)	134 (94%)	7 (5%)	1 (1%)	26	66
1	AZ	142/148 (96%)	134 (94%)	7 (5%)	1 (1%)	26	66
1	Aa	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Ab	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Ac	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Ad	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Ae	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Af	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Ag	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Ah	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Ai	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Aj	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Ak	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Al	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	Am	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	An	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	Ao	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	Ap	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Aq	142/148 (96%)	137 (96%)	4 (3%)	1 (1%)	26	66
1	Ar	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	As	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	At	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Au	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Av	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
1	Aw	142/148 (96%)	135 (95%)	6 (4%)	1 (1%)	26	66
1	Ax	142/148 (96%)	136 (96%)	5 (4%)	1 (1%)	26	66
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%)	30	68

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%)	31	70
1	A1	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	A2	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A3	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	A4	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A5	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A6	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A7	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A8	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	A9	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AA	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AB	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AC	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AD	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AE	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AF	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AG	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AH	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AI	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AJ	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AK	126/130 (97%)	121 (96%)	5 (4%)	38	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AL	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AM	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AN	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AO	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AP	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AQ	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AR	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AS	126/130 (97%)	122 (97%)	4 (3%)	46	79
1	AT	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AU	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AV	126/130 (97%)	119 (94%)	7 (6%)	26	65
1	AW	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AX	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	AY	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	AZ	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Aa	126/130 (97%)	122 (97%)	4 (3%)	46	79
1	Ab	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Ac	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ad	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ae	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Af	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ag	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ah	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ai	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Aj	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ak	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Al	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Am	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	An	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Ao	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Ap	126/130 (97%)	120 (95%)	6 (5%)	31	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aq	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Ar	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	As	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	At	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Au	126/130 (97%)	121 (96%)	5 (4%)	38	74
1	Av	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Aw	126/130 (97%)	120 (95%)	6 (5%)	31	70
1	Ax	126/130 (97%)	120 (95%)	6 (5%)	31	70
2	B0	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B1	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B2	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B3	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B4	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B5	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B6	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B7	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B8	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	B9	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BA	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BB	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BC	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BD	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BE	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BF	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BG	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BH	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BI	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BJ	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BK	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BL	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BM	22/51 (43%)	21 (96%)	1 (4%)	34	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	BN	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BO	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BP	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BQ	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BR	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BS	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BT	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BU	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BV	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BW	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BX	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BY	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	BZ	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Ba	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bb	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bc	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bd	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Be	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bf	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bg	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bh	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bi	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bj	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bk	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bl	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bm	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bn	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bo	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bp	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bq	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Br	22/51 (43%)	21 (96%)	1 (4%)	34	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bs	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bt	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bu	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bv	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bw	22/51 (43%)	21 (96%)	1 (4%)	34	72
2	Bx	22/51 (43%)	21 (96%)	1 (4%)	34	72
All	All	8880/10860 (82%)	8500 (96%)	380 (4%)	35	72

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 molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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.

No monomer is involved in short contacts.

## 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%)	-0.47	1 (0%) 89 86	19, 36, 57, 67	0
1	A1	144/148 (97%)	-0.40	0 100 100	18, 36, 58, 67	0
1	A2	144/148 (97%)	-0.46	1 (0%) 89 86	19, 36, 58, 67	0
1	A3	144/148 (97%)	-0.37	1 (0%) 89 86	18, 35, 57, 66	0
1	A4	144/148 (97%)	-0.20	3 (2%) 67 60	21, 38, 60, 68	0
1	A5	144/148 (97%)	-0.40	0 100 100	18, 35, 57, 65	0
1	A6	144/148 (97%)	-0.49	0 100 100	19, 37, 59, 67	0
1	A7	144/148 (97%)	-0.40	0 100 100	18, 36, 57, 66	0
1	A8	144/148 (97%)	-0.48	0 100 100	18, 37, 59, 66	0
1	A9	144/148 (97%)	-0.43	0 100 100	16, 35, 57, 66	0
1	AA	144/148 (97%)	-0.27	3 (2%) 67 60	23, 38, 60, 68	0
1	AB	144/148 (97%)	-0.45	0 100 100	18, 37, 59, 66	0
1	AC	144/148 (97%)	-0.38	2 (1%) 78 73	20, 38, 59, 68	0
1	AD	144/148 (97%)	-0.37	0 100 100	15, 34, 57, 65	0
1	AE	144/148 (97%)	-0.48	1 (0%) 89 86	21, 37, 59, 68	0
1	AF	144/148 (97%)	-0.46	0 100 100	18, 36, 57, 67	0
1	AG	144/148 (97%)	-0.29	1 (0%) 89 86	21, 38, 59, 68	0
1	AH	144/148 (97%)	-0.41	1 (0%) 89 86	19, 36, 58, 67	0
1	AI	144/148 (97%)	-0.39	2 (1%) 78 73	20, 38, 59, 68	0
1	AJ	144/148 (97%)	-0.39	0 100 100	17, 34, 57, 66	0
1	AK	144/148 (97%)	-0.51	0 100 100	20, 37, 58, 67	0
1	AL	144/148 (97%)	-0.43	0 100 100	17, 34, 57, 66	0
1	AM	144/148 (97%)	-0.38	1 (0%) 89 86	22, 39, 59, 68	0
1	AN	144/148 (97%)	-0.47	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%)	-0.45	0 100 100	20, 38, 60, 68	0
1	AP	144/148 (97%)	-0.39	0 100 100	15, 35, 58, 67	0
1	AQ	144/148 (97%)	-0.52	0 100 100	20, 37, 58, 66	0
1	AR	144/148 (97%)	-0.42	0 100 100	18, 36, 58, 67	0
1	AS	144/148 (97%)	-0.34	1 (0%) 89 86	21, 38, 59, 68	0
1	AT	144/148 (97%)	-0.45	0 100 100	18, 36, 57, 66	0
1	AU	144/148 (97%)	-0.49	0 100 100	20, 36, 58, 67	0
1	AV	144/148 (97%)	-0.47	0 100 100	17, 36, 58, 66	0
1	AW	144/148 (97%)	-0.46	0 100 100	20, 37, 58, 67	0
1	AX	144/148 (97%)	-0.43	0 100 100	16, 35, 58, 66	0
1	AY	144/148 (97%)	-0.26	2 (1%) 78 73	22, 38, 59, 68	0
1	AZ	144/148 (97%)	-0.42	0 100 100	19, 36, 57, 66	0
1	Aa	144/148 (97%)	-0.44	1 (0%) 89 86	19, 38, 59, 67	0
1	Ab	144/148 (97%)	-0.48	0 100 100	17, 35, 57, 66	0
1	Ac	144/148 (97%)	-0.50	0 100 100	21, 38, 59, 68	0
1	Ad	144/148 (97%)	-0.44	0 100 100	16, 34, 57, 66	0
1	Ae	144/148 (97%)	-0.46	0 100 100	20, 37, 59, 67	0
1	Af	144/148 (97%)	-0.41	1 (0%) 89 86	20, 37, 59, 67	0
1	Ag	144/148 (97%)	-0.42	1 (0%) 89 86	20, 37, 58, 67	0
1	Ah	144/148 (97%)	-0.41	0 100 100	18, 35, 57, 66	0
1	Ai	144/148 (97%)	-0.40	1 (0%) 89 86	21, 38, 59, 68	0
1	Aj	144/148 (97%)	-0.42	0 100 100	17, 35, 57, 66	0
1	Ak	144/148 (97%)	-0.48	0 100 100	19, 37, 59, 67	0
1	Al	144/148 (97%)	-0.49	1 (0%) 89 86	20, 37, 59, 68	0
1	Am	144/148 (97%)	-0.41	1 (0%) 89 86	19, 36, 58, 68	0
1	An	144/148 (97%)	-0.41	0 100 100	17, 35, 58, 66	0
1	Ao	144/148 (97%)	-0.46	0 100 100	21, 38, 59, 68	0
1	Ap	144/148 (97%)	-0.44	0 100 100	16, 35, 58, 66	0
1	Aq	144/148 (97%)	-0.46	0 100 100	19, 37, 59, 68	0
1	Ar	144/148 (97%)	-0.44	1 (0%) 89 86	19, 37, 58, 67	0
1	As	144/148 (97%)	-0.47	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%)	-0.40	0 100 100	18, 35, 57, 66	0
1	Au	144/148 (97%)	-0.45	0 100 100	20, 36, 58, 68	0
1	Av	144/148 (97%)	-0.40	0 100 100	19, 37, 58, 67	0
1	Aw	144/148 (97%)	-0.42	0 100 100	18, 36, 58, 66	0
1	Ax	144/148 (97%)	-0.39	0 100 100	17, 35, 57, 66	0
2	B0	25/63 (39%)	0.99	3 (12%) 6 5	55, 91, 126, 136	0
2	B1	25/63 (39%)	1.24	5 (20%) 1 1	56, 92, 126, 136	0
2	B2	25/63 (39%)	1.20	6 (24%) 1 1	55, 91, 126, 135	0
2	B3	25/63 (39%)	1.14	3 (12%) 6 5	55, 90, 125, 135	0
2	B4	25/63 (39%)	1.55	9 (36%) 0 1	58, 93, 126, 136	0
2	B5	25/63 (39%)	1.33	5 (20%) 1 1	55, 90, 125, 136	0
2	B6	25/63 (39%)	0.96	4 (16%) 3 2	57, 91, 126, 136	0
2	B7	25/63 (39%)	1.30	3 (12%) 6 5	55, 91, 126, 136	0
2	B8	25/63 (39%)	1.38	5 (20%) 1 1	55, 91, 126, 136	0
2	B9	25/63 (39%)	1.30	5 (20%) 1 1	55, 91, 125, 135	0
2	BA	25/63 (39%)	1.38	7 (28%) 1 1	58, 92, 126, 136	0
2	BB	25/63 (39%)	1.06	5 (20%) 1 1	57, 92, 126, 136	0
2	BC	25/63 (39%)	1.38	8 (32%) 1 1	57, 92, 126, 135	0
2	BD	25/63 (39%)	1.71	5 (20%) 1 1	54, 89, 125, 136	0
2	BE	25/63 (39%)	1.34	7 (28%) 1 1	57, 92, 126, 136	0
2	BF	25/63 (39%)	1.28	5 (20%) 1 1	56, 91, 126, 135	0
2	BG	25/63 (39%)	1.81	9 (36%) 0 1	57, 93, 126, 135	0
2	BH	25/63 (39%)	1.20	5 (20%) 1 1	55, 90, 126, 136	0
2	BI	25/63 (39%)	1.26	5 (20%) 1 1	57, 92, 126, 135	0
2	BJ	25/63 (39%)	1.19	5 (20%) 1 1	54, 91, 125, 135	0
2	BK	25/63 (39%)	1.43	7 (28%) 1 1	57, 92, 126, 135	0
2	BL	25/63 (39%)	1.23	4 (16%) 3 2	54, 89, 125, 135	0
2	BM	25/63 (39%)	1.80	8 (32%) 1 1	58, 93, 126, 136	0
2	BN	25/63 (39%)	1.33	5 (20%) 1 1	55, 92, 125, 135	0
2	BO	25/63 (39%)	1.33	9 (36%) 0 1	58, 93, 126, 136	0
2	BP	25/63 (39%)	1.27	3 (12%) 6 5	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%)	1.31	4 (16%)	3	2	56, 91, 126, 136	0
2	BR	25/63 (39%)	1.30	5 (20%)	1	1	55, 92, 125, 136	0
2	BS	25/63 (39%)	1.36	6 (24%)	1	1	57, 93, 126, 136	0
2	BT	25/63 (39%)	1.44	5 (20%)	1	1	56, 92, 126, 136	0
2	BU	25/63 (39%)	1.22	7 (28%)	1	1	56, 92, 126, 136	0
2	BV	25/63 (39%)	1.30	7 (28%)	1	1	56, 91, 126, 136	0
2	BW	25/63 (39%)	1.27	5 (20%)	1	1	57, 92, 126, 136	0
2	BX	25/63 (39%)	1.23	4 (16%)	3	2	55, 91, 126, 136	0
2	BY	25/63 (39%)	1.69	9 (36%)	0	1	58, 92, 126, 136	0
2	BZ	25/63 (39%)	1.12	3 (12%)	6	5	54, 90, 125, 136	0
2	Ba	25/63 (39%)	1.33	7 (28%)	1	1	56, 91, 126, 136	0
2	Bb	25/63 (39%)	1.23	4 (16%)	3	2	54, 90, 125, 135	0
2	Bc	25/63 (39%)	1.40	8 (32%)	1	1	57, 92, 125, 135	0
2	Bd	25/63 (39%)	1.06	4 (16%)	3	2	54, 91, 125, 136	0
2	Be	25/63 (39%)	1.31	6 (24%)	1	1	56, 91, 126, 136	0
2	Bf	25/63 (39%)	1.88	6 (24%)	1	1	58, 92, 126, 136	0
2	Bg	25/63 (39%)	2.14	9 (36%)	0	1	56, 92, 126, 135	0
2	Bh	25/63 (39%)	1.27	5 (20%)	1	1	54, 91, 126, 135	0
2	Bi	25/63 (39%)	1.45	6 (24%)	1	1	57, 92, 126, 136	0
2	Bj	25/63 (39%)	1.42	3 (12%)	6	5	54, 90, 125, 136	0
2	Bk	25/63 (39%)	1.23	3 (12%)	6	5	56, 91, 125, 136	0
2	Bl	25/63 (39%)	1.29	5 (20%)	1	1	56, 92, 125, 135	0
2	Bm	25/63 (39%)	1.30	4 (16%)	3	2	56, 92, 126, 136	0
2	Bn	25/63 (39%)	1.06	3 (12%)	6	5	55, 91, 126, 136	0
2	Bo	25/63 (39%)	1.06	5 (20%)	1	1	57, 91, 126, 136	0
2	Bp	25/63 (39%)	1.63	4 (16%)	3	2	54, 89, 125, 136	0
2	Bq	25/63 (39%)	1.56	5 (20%)	1	1	56, 92, 126, 136	0
2	Br	25/63 (39%)	1.52	9 (36%)	0	1	57, 92, 126, 135	0
2	Bs	25/63 (39%)	1.04	3 (12%)	6	5	55, 90, 125, 136	0
2	Bt	25/63 (39%)	1.28	3 (12%)	6	5	54, 91, 125, 136	0
2	Bu	25/63 (39%)	1.15	6 (24%)	1	1	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%)	0.90	3 (12%) 6 5	55, 91, 125, 136	0
2	Bw	25/63 (39%)	1.34	3 (12%) 6 5	55, 91, 125, 136	0
2	Bx	25/63 (39%)	1.33	5 (20%) 1 1	54, 89, 126, 135	0
All	All	10140/12660 (80%)	-0.16	346 (3%) 49 42	15, 39, 106, 136	0

The worst 5 of 346 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Bf	41	PRO	11.9
2	BR	41	PRO	11.2
2	Bp	41	PRO	10.9
2	B7	41	PRO	10.4
2	Bq	41	PRO	9.7

## 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	Ac	302	1/1	0.84	1.93	84.72	68,68,68,68	0
3	MG	AN	301	1/1	0.96	1.30	80.48	69,69,69,69	0
3	MG	AJ	301	1/1	0.91	1.11	73.22	46,46,46,46	0
3	MG	An	301	1/1	0.94	1.01	72.37	41,41,41,41	0
3	MG	Aq	301	1/1	0.88	0.95	71.30	45,45,45,45	0
3	MG	AO	301	1/1	0.86	1.37	70.20	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A9	302	1/1	0.84	1.21	64.13	62,62,62,62	0
3	MG	AR	301	1/1	0.84	1.10	58.87	59,59,59,59	0
3	MG	Aw	302	1/1	0.90	0.89	48.86	38,38,38,38	0
3	MG	A5	302	1/1	0.92	1.05	43.97	36,36,36,36	0
3	MG	AA	1002	1/1	0.80	1.50	42.36	63,63,63,63	0
3	MG	A7	301	1/1	0.87	1.18	38.13	42,42,42,42	0
3	MG	A6	302	1/1	0.89	1.00	36.12	45,45,45,45	0
3	MG	Am	301	1/1	0.80	0.99	36.05	49,49,49,49	0
3	MG	AQ	302	1/1	0.83	0.98	35.10	59,59,59,59	0
3	MG	Av	301	1/1	0.89	0.80	34.89	35,35,35,35	0
3	MG	Ar	301	1/1	0.84	1.05	34.49	61,61,61,61	0
3	MG	Ak	301	1/1	0.74	0.56	34.41	37,37,37,37	0
3	MG	A8	302	1/1	0.71	1.35	33.34	54,54,54,54	0
3	MG	A4	302	1/1	0.85	1.04	32.52	73,73,73,73	0
3	MG	Ap	301	1/1	0.95	0.74	31.25	32,32,32,32	0
3	MG	AC	301	1/1	0.75	0.71	29.90	46,46,46,46	0
3	MG	Ah	301	1/1	0.72	0.53	28.08	41,41,41,41	0
3	MG	AB	301	1/1	0.89	0.40	26.88	35,35,35,35	0
3	MG	AD	301	1/1	0.82	0.42	23.19	25,25,25,25	0
3	MG	AQ	301	1/1	0.78	0.75	22.14	25,25,25,25	0
3	MG	A9	301	1/1	0.72	0.46	19.60	37,37,37,37	0
3	MG	AF	301	1/1	0.74	0.47	19.02	28,28,28,28	0
3	MG	Ac	301	1/1	0.85	0.52	18.02	43,43,43,43	0
3	MG	A6	301	1/1	0.76	0.41	11.95	53,53,53,53	0
3	MG	A8	301	1/1	0.85	0.50	8.67	22,22,22,22	0
3	MG	Ad	301	1/1	0.86	0.34	8.16	17,17,17,17	0
3	MG	Aw	301	1/1	0.83	0.30	8.08	20,20,20,20	0
3	MG	A1	301	1/1	0.72	0.39	7.84	20,20,20,20	0
3	MG	A5	301	1/1	0.83	0.35	7.52	11,11,11,11	0
3	MG	A4	301	1/1	0.72	0.38	6.58	44,44,44,44	0
3	MG	As	301	1/1	0.65	0.28	6.52	21,21,21,21	0
3	MG	Aa	301	1/1	0.88	0.28	5.51	28,28,28,28	0
3	MG	AA	1001	1/1	0.71	0.35	5.06	46,46,46,46	0
3	MG	Af	301	1/1	0.92	0.24	3.53	23,23,23,23	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.