



wwPDB X-ray Structure Validation Summary Report

Mar 13, 2014 – 06:06 AM GMT

PDB ID : 4CBO
Title : Crystal structure of Complement Factor D mutant R202A after ensemble refinement
Authors : Forneris, F.; Burnley, B.T.; Gros, P.
Deposited on : 2013-10-15
Resolution : 1.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

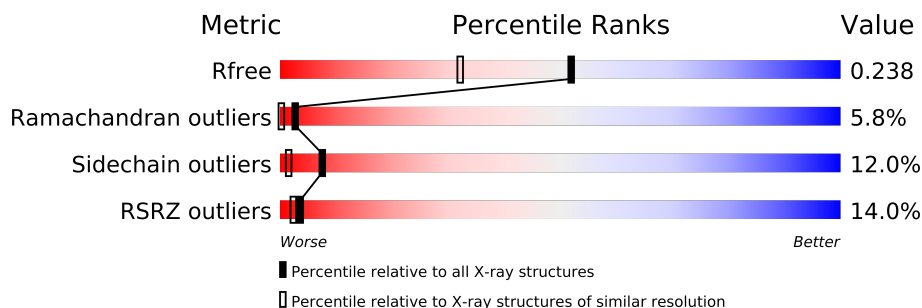
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
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) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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	3513 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 ≥ 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	1-A	228	
1	1-B	228	
1	10-A	228	
1	10-B	228	
1	11-A	228	
1	11-B	228	
1	12-A	228	
1	12-B	228	
1	13-A	228	
1	13-B	228	
1	14-A	228	
1	14-B	228	
1	15-A	228	
1	15-B	228	
1	16-A	228	
1	16-B	228	

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Mol	Chain	Length	Quality of chain
1	17-A	228	
1	17-B	228	
1	18-A	228	
1	18-B	228	
1	19-A	228	
1	19-B	228	
1	2-A	228	
1	2-B	228	
1	20-A	228	
1	20-B	228	
1	21-A	228	
1	21-B	228	
1	22-A	228	
1	22-B	228	
1	23-A	228	
1	23-B	228	
1	24-A	228	
1	24-B	228	
1	25-A	228	
1	25-B	228	
1	26-A	228	
1	26-B	228	
1	27-A	228	
1	27-B	228	
1	28-A	228	
1	28-B	228	
1	29-A	228	
1	29-B	228	
1	3-A	228	
1	3-B	228	
1	30-A	228	
1	30-B	228	
1	31-A	228	
1	31-B	228	
1	32-A	228	
1	32-B	228	
1	33-A	228	
1	33-B	228	
1	34-A	228	
1	34-B	228	
1	35-A	228	
1	35-B	228	

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Mol	Chain	Length	Quality of chain
1	36-A	228	
1	36-B	228	
1	37-A	228	
1	37-B	228	
1	38-A	228	
1	38-B	228	
1	39-A	228	
1	39-B	228	
1	4-A	228	
1	4-B	228	
1	40-A	228	
1	40-B	228	
1	41-A	228	
1	41-B	228	
1	42-A	228	
1	42-B	228	
1	43-A	228	
1	43-B	228	
1	44-A	228	
1	44-B	228	
1	45-A	228	
1	45-B	228	
1	46-A	228	
1	46-B	228	
1	47-A	228	
1	47-B	228	
1	48-A	228	
1	48-B	228	
1	49-A	228	
1	49-B	228	
1	5-A	228	
1	5-B	228	
1	50-A	228	
1	50-B	228	
1	51-A	228	
1	51-B	228	
1	52-A	228	
1	52-B	228	
1	53-A	228	
1	53-B	228	
1	54-A	228	
1	54-B	228	










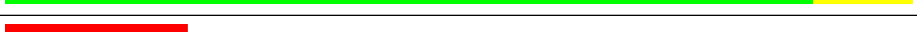

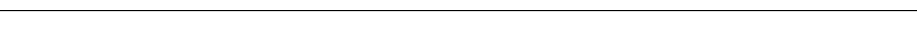
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Mol	Chain	Length	Quality of chain
1	55-A	228	
1	55-B	228	
1	56-A	228	
1	56-B	228	
1	57-A	228	
1	57-B	228	
1	58-A	228	
1	58-B	228	
1	59-A	228	
1	59-B	228	
1	6-A	228	
1	6-B	228	
1	60-A	228	
1	60-B	228	
1	61-A	228	
1	61-B	228	
1	62-A	228	
1	62-B	228	
1	63-A	228	
1	63-B	228	
1	64-A	228	
1	64-B	228	
1	65-A	228	
1	65-B	228	
1	66-A	228	
1	66-B	228	
1	67-A	228	
1	67-B	228	
1	68-A	228	
1	68-B	228	
1	69-A	228	
1	69-B	228	
1	7-A	228	
1	7-B	228	
1	70-A	228	
1	70-B	228	
1	71-A	228	
1	71-B	228	
1	72-A	228	
1	72-B	228	
1	73-A	228	
1	73-B	228	

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Mol	Chain	Length	Quality of chain
1	74-A	228	
1	74-B	228	
1	75-A	228	
1	75-B	228	
1	76-A	228	
1	76-B	228	
1	77-A	228	
1	77-B	228	
1	8-A	228	
1	8-B	228	
1	9-A	228	
1	9-B	228	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 546299 atoms, of which 263032 are hydrogens 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 COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	3-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	4-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	5-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	6-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	7-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	8-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	9-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	10-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	11-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	12-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	13-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	14-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	15-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	16-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	17-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	18-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	19-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	20-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	21-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	22-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	23-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	24-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	25-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	26-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	27-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	28-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	29-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	30-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	31-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	32-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	33-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	34-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	35-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	36-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	37-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	38-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	39-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	40-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	41-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	42-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	43-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	44-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	45-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	46-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	47-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	48-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	49-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	50-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	51-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	52-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	53-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	54-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	55-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	56-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	57-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	58-A	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	59-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	66-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-A	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	1-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	2-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	3-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	4-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	5-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	6-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	7-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	8-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	9-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	10-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	11-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	12-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	13-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	14-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	15-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	16-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	17-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	18-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	19-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	20-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	21-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	22-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	23-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	24-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	25-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	26-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	27-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	28-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	29-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	30-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	31-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	32-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	33-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	34-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	35-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	36-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	37-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	38-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	39-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	40-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	41-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	42-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	43-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0
1	44-B	228	Total 3406	C 1055	H 1700	N 322	O 319	S 10	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	45-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	46-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	47-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	48-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	49-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	50-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	51-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	52-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	53-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	54-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	55-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	56-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	57-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	58-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	59-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	60-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	61-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	62-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	63-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	64-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	65-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	66-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	67-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	68-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	69-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	70-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	71-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	72-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	73-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	74-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	75-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	76-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			
1	77-B	228	Total	C	H	N	O	S	0	0	0
			3406	1055	1700	322	319	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	ALA	ARG	ENGINEERED MUTATION	UNP P00746
B	202	ALA	ARG	ENGINEERED MUTATION	UNP P00746

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	2-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	3-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	4-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	5-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	6-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	7-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	8-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	9-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	10-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	11-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	12-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	13-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	14-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	15-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	16-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	17-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	18-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	19-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	20-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	21-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	22-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	23-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	24-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	25-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	26-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	27-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	28-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	29-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	30-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	31-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	32-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	33-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	34-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	35-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	36-A	1	Total 14	C 3	H 8	O 3	0	0
2	37-A	1	Total 14	C 3	H 8	O 3	0	0
2	38-A	1	Total 14	C 3	H 8	O 3	0	0
2	39-A	1	Total 14	C 3	H 8	O 3	0	0
2	40-A	1	Total 14	C 3	H 8	O 3	0	0
2	41-A	1	Total 14	C 3	H 8	O 3	0	0
2	42-A	1	Total 14	C 3	H 8	O 3	0	0
2	43-A	1	Total 14	C 3	H 8	O 3	0	0
2	44-A	1	Total 14	C 3	H 8	O 3	0	0
2	45-A	1	Total 14	C 3	H 8	O 3	0	0
2	46-A	1	Total 14	C 3	H 8	O 3	0	0
2	47-A	1	Total 14	C 3	H 8	O 3	0	0
2	48-A	1	Total 14	C 3	H 8	O 3	0	0
2	49-A	1	Total 14	C 3	H 8	O 3	0	0
2	50-A	1	Total 14	C 3	H 8	O 3	0	0
2	51-A	1	Total 14	C 3	H 8	O 3	0	0
2	52-A	1	Total 14	C 3	H 8	O 3	0	0
2	53-A	1	Total 14	C 3	H 8	O 3	0	0
2	54-A	1	Total 14	C 3	H 8	O 3	0	0
2	55-A	1	Total 14	C 3	H 8	O 3	0	0
2	56-A	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	57-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	58-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	59-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	60-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	61-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	62-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	63-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	64-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-A	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-A	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1-B	1	Total 14	C 3	H 8	O 3	0	0
2	2-B	1	Total 14	C 3	H 8	O 3	0	0
2	3-B	1	Total 14	C 3	H 8	O 3	0	0
2	4-B	1	Total 14	C 3	H 8	O 3	0	0
2	5-B	1	Total 14	C 3	H 8	O 3	0	0
2	6-B	1	Total 14	C 3	H 8	O 3	0	0
2	7-B	1	Total 14	C 3	H 8	O 3	0	0
2	8-B	1	Total 14	C 3	H 8	O 3	0	0
2	9-B	1	Total 14	C 3	H 8	O 3	0	0
2	10-B	1	Total 14	C 3	H 8	O 3	0	0
2	11-B	1	Total 14	C 3	H 8	O 3	0	0
2	12-B	1	Total 14	C 3	H 8	O 3	0	0
2	13-B	1	Total 14	C 3	H 8	O 3	0	0
2	14-B	1	Total 14	C 3	H 8	O 3	0	0
2	15-B	1	Total 14	C 3	H 8	O 3	0	0
2	16-B	1	Total 14	C 3	H 8	O 3	0	0
2	17-B	1	Total 14	C 3	H 8	O 3	0	0
2	18-B	1	Total 14	C 3	H 8	O 3	0	0
2	19-B	1	Total 14	C 3	H 8	O 3	0	0
2	20-B	1	Total 14	C 3	H 8	O 3	0	0
2	21-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	22-B	1	Total 14	C 3	H 8	O 3	0	0
2	23-B	1	Total 14	C 3	H 8	O 3	0	0
2	24-B	1	Total 14	C 3	H 8	O 3	0	0
2	25-B	1	Total 14	C 3	H 8	O 3	0	0
2	26-B	1	Total 14	C 3	H 8	O 3	0	0
2	27-B	1	Total 14	C 3	H 8	O 3	0	0
2	28-B	1	Total 14	C 3	H 8	O 3	0	0
2	29-B	1	Total 14	C 3	H 8	O 3	0	0
2	30-B	1	Total 14	C 3	H 8	O 3	0	0
2	31-B	1	Total 14	C 3	H 8	O 3	0	0
2	32-B	1	Total 14	C 3	H 8	O 3	0	0
2	33-B	1	Total 14	C 3	H 8	O 3	0	0
2	34-B	1	Total 14	C 3	H 8	O 3	0	0
2	35-B	1	Total 14	C 3	H 8	O 3	0	0
2	36-B	1	Total 14	C 3	H 8	O 3	0	0
2	37-B	1	Total 14	C 3	H 8	O 3	0	0
2	38-B	1	Total 14	C 3	H 8	O 3	0	0
2	39-B	1	Total 14	C 3	H 8	O 3	0	0
2	40-B	1	Total 14	C 3	H 8	O 3	0	0
2	41-B	1	Total 14	C 3	H 8	O 3	0	0
2	42-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	43-B	1	Total 14	C 3	H 8	O 3	0	0
2	44-B	1	Total 14	C 3	H 8	O 3	0	0
2	45-B	1	Total 14	C 3	H 8	O 3	0	0
2	46-B	1	Total 14	C 3	H 8	O 3	0	0
2	47-B	1	Total 14	C 3	H 8	O 3	0	0
2	48-B	1	Total 14	C 3	H 8	O 3	0	0
2	49-B	1	Total 14	C 3	H 8	O 3	0	0
2	50-B	1	Total 14	C 3	H 8	O 3	0	0
2	51-B	1	Total 14	C 3	H 8	O 3	0	0
2	52-B	1	Total 14	C 3	H 8	O 3	0	0
2	53-B	1	Total 14	C 3	H 8	O 3	0	0
2	54-B	1	Total 14	C 3	H 8	O 3	0	0
2	55-B	1	Total 14	C 3	H 8	O 3	0	0
2	56-B	1	Total 14	C 3	H 8	O 3	0	0
2	57-B	1	Total 14	C 3	H 8	O 3	0	0
2	58-B	1	Total 14	C 3	H 8	O 3	0	0
2	59-B	1	Total 14	C 3	H 8	O 3	0	0
2	60-B	1	Total 14	C 3	H 8	O 3	0	0
2	61-B	1	Total 14	C 3	H 8	O 3	0	0
2	62-B	1	Total 14	C 3	H 8	O 3	0	0
2	63-B	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	64-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	65-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	66-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	67-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	68-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	69-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	70-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	71-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	72-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	73-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	74-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	75-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	76-B	1	Total	C	H	O	0	0
			14	3	8	3		
2	77-B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1-A	148	Total	O	0	0
			148	148		
3	2-A	139	Total	O	0	0
			139	139		
3	3-A	142	Total	O	0	0
			142	142		
3	4-A	129	Total	O	0	0
			129	129		
3	5-A	128	Total	O	0	1
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	6-A	135	Total 136	O 136	0	1
3	7-A	134	Total 134	O 134	0	0
3	8-A	136	Total 136	O 136	0	0
3	9-A	138	Total 138	O 138	0	0
3	10-A	135	Total 135	O 135	0	0
3	11-A	123	Total 123	O 123	0	0
3	12-A	145	Total 145	O 145	0	0
3	13-A	164	Total 165	O 165	0	1
3	14-A	157	Total 157	O 157	0	0
3	15-A	142	Total 142	O 142	0	0
3	16-A	135	Total 135	O 135	0	0
3	17-A	142	Total 142	O 142	0	0
3	18-A	147	Total 147	O 147	0	0
3	19-A	127	Total 127	O 127	0	0
3	20-A	131	Total 131	O 131	0	0
3	21-A	144	Total 144	O 144	0	0
3	22-A	142	Total 143	O 143	0	1
3	23-A	142	Total 142	O 142	0	0
3	24-A	127	Total 127	O 127	0	0
3	25-A	136	Total 137	O 137	0	1
3	26-A	144	Total 145	O 145	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	27-A	139	Total 139	O 139	0	0
3	28-A	136	Total 137	O 137	0	1
3	29-A	134	Total 135	O 135	0	1
3	30-A	149	Total 149	O 149	0	0
3	31-A	146	Total 146	O 146	0	0
3	32-A	135	Total 135	O 135	0	0
3	33-A	133	Total 133	O 133	0	0
3	34-A	139	Total 139	O 139	0	0
3	35-A	125	Total 125	O 125	0	0
3	36-A	130	Total 130	O 130	0	0
3	37-A	138	Total 138	O 138	0	0
3	38-A	133	Total 134	O 134	0	1
3	39-A	130	Total 130	O 130	0	0
3	40-A	127	Total 128	O 128	0	1
3	41-A	139	Total 139	O 139	0	0
3	42-A	128	Total 128	O 128	0	0
3	43-A	154	Total 155	O 155	0	1
3	44-A	143	Total 143	O 143	0	0
3	45-A	140	Total 140	O 140	0	0
3	46-A	131	Total 131	O 131	0	0
3	47-A	127	Total 127	O 127	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	48-A	141	Total 141	O 141	0	0
3	49-A	121	Total 121	O 121	0	0
3	50-A	138	Total 139	O 139	0	1
3	51-A	137	Total 137	O 137	0	0
3	52-A	145	Total 145	O 145	0	0
3	53-A	141	Total 141	O 141	0	0
3	54-A	137	Total 137	O 137	0	0
3	55-A	135	Total 136	O 136	0	1
3	56-A	152	Total 153	O 153	0	1
3	57-A	124	Total 124	O 124	0	0
3	58-A	133	Total 133	O 133	0	0
3	59-A	142	Total 143	O 143	0	1
3	60-A	132	Total 132	O 132	0	0
3	61-A	138	Total 138	O 138	0	0
3	62-A	136	Total 137	O 137	0	1
3	63-A	151	Total 151	O 151	0	0
3	64-A	142	Total 142	O 142	0	0
3	65-A	148	Total 149	O 149	0	1
3	66-A	135	Total 135	O 135	0	0
3	67-A	143	Total 143	O 143	0	0
3	68-A	137	Total 137	O 137	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	69-A	131	Total 131	O 131	0	0
3	70-A	136	Total 136	O 136	0	0
3	71-A	137	Total 138	O 138	0	1
3	72-A	135	Total 135	O 135	0	0
3	73-A	134	Total 134	O 134	0	0
3	74-A	153	Total 153	O 153	0	0
3	75-A	147	Total 147	O 147	0	0
3	76-A	145	Total 145	O 145	0	0
3	77-A	131	Total 131	O 131	0	0
3	1-B	113	Total 113	O 113	0	0
3	2-B	122	Total 122	O 122	0	0
3	3-B	96	Total 96	O 96	0	0
3	4-B	108	Total 108	O 108	0	0
3	5-B	109	Total 109	O 109	0	0
3	6-B	111	Total 111	O 111	0	0
3	7-B	111	Total 111	O 111	0	0
3	8-B	104	Total 104	O 104	0	0
3	9-B	118	Total 119	O 119	0	1
3	10-B	117	Total 117	O 117	0	0
3	11-B	118	Total 118	O 118	0	0
3	12-B	114	Total 115	O 115	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	13-B	109	Total 109	O 109	0	0
3	14-B	115	Total 115	O 115	0	0
3	15-B	113	Total 113	O 113	0	0
3	16-B	117	Total 117	O 117	0	0
3	17-B	121	Total 122	O 122	0	1
3	18-B	111	Total 111	O 111	0	0
3	19-B	117	Total 117	O 117	0	0
3	20-B	122	Total 123	O 123	0	1
3	21-B	103	Total 103	O 103	0	0
3	22-B	122	Total 122	O 122	0	0
3	23-B	113	Total 113	O 113	0	0
3	24-B	116	Total 116	O 116	0	0
3	25-B	120	Total 120	O 120	0	0
3	26-B	114	Total 114	O 114	0	0
3	27-B	114	Total 114	O 114	0	0
3	28-B	123	Total 123	O 123	0	0
3	29-B	132	Total 132	O 132	0	0
3	30-B	115	Total 115	O 115	0	0
3	31-B	117	Total 117	O 117	0	0
3	32-B	127	Total 127	O 127	0	0
3	33-B	119	Total 119	O 119	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	34-B	109	Total 109	O 109	0	0
3	35-B	102	Total 102	O 102	0	0
3	36-B	119	Total 120	O 120	0	1
3	37-B	110	Total 110	O 110	0	0
3	38-B	118	Total 118	O 118	0	0
3	39-B	112	Total 112	O 112	0	0
3	40-B	118	Total 118	O 118	0	0
3	41-B	106	Total 106	O 106	0	0
3	42-B	123	Total 124	O 124	0	1
3	43-B	125	Total 125	O 125	0	0
3	44-B	118	Total 118	O 118	0	0
3	45-B	108	Total 108	O 108	0	0
3	46-B	105	Total 105	O 105	0	0
3	47-B	117	Total 118	O 118	0	1
3	48-B	128	Total 129	O 129	0	1
3	49-B	109	Total 109	O 109	0	0
3	50-B	111	Total 111	O 111	0	0
3	51-B	130	Total 131	O 131	0	1
3	52-B	119	Total 119	O 119	0	0
3	53-B	113	Total 113	O 113	0	0
3	54-B	109	Total 109	O 109	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	55-B	120	Total 120	O 120	0	0
3	56-B	127	Total 127	O 127	0	0
3	57-B	122	Total 122	O 122	0	0
3	58-B	121	Total 122	O 122	0	1
3	59-B	117	Total 117	O 117	0	0
3	60-B	116	Total 116	O 116	0	0
3	61-B	118	Total 119	O 119	0	1
3	62-B	121	Total 121	O 121	0	0
3	63-B	122	Total 123	O 123	0	1
3	64-B	121	Total 121	O 121	0	0
3	65-B	128	Total 128	O 128	0	0
3	66-B	112	Total 112	O 112	0	0
3	67-B	124	Total 125	O 125	0	1
3	68-B	126	Total 126	O 126	0	0
3	69-B	112	Total 112	O 112	0	0
3	70-B	122	Total 123	O 123	0	1
3	71-B	122	Total 122	O 122	0	0
3	72-B	121	Total 121	O 121	0	0
3	73-B	131	Total 132	O 132	0	1
3	74-B	113	Total 113	O 113	0	0
3	75-B	111	Total 111	O 111	0	0

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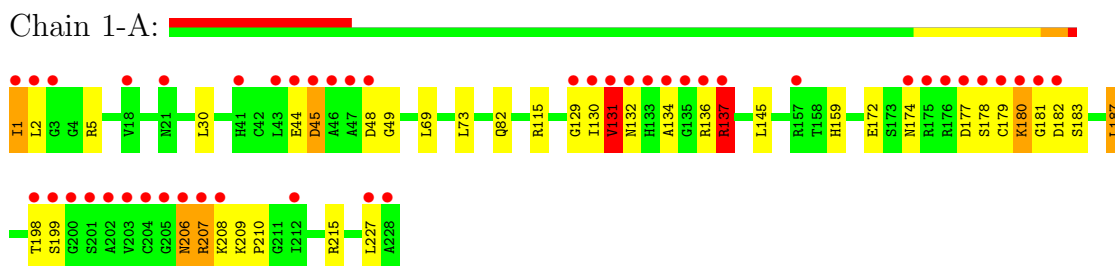
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	76-B	105	Total 105	O 105	0	0
3	77-B	119	Total 119	O 119	0	0

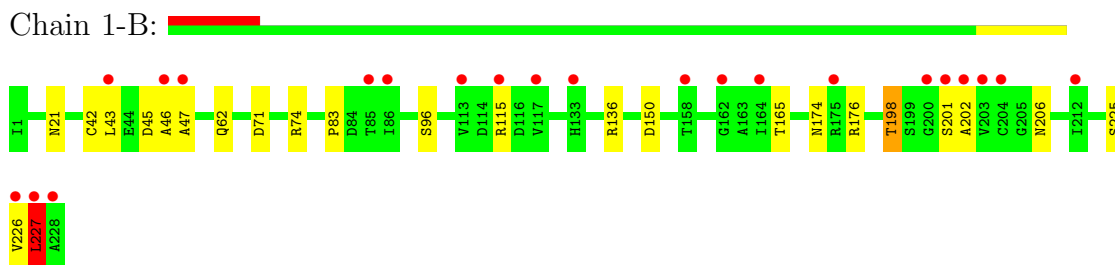
3 Residue-property plots

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.

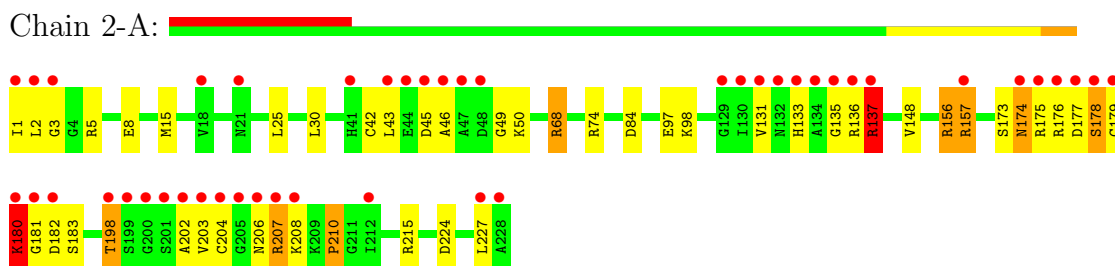
• Molecule 1: COMPLEMENT FACTOR D



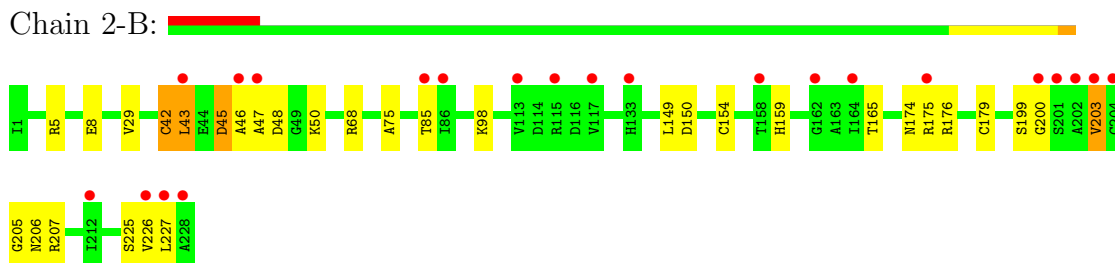
• Molecule 1: COMPLEMENT FACTOR D



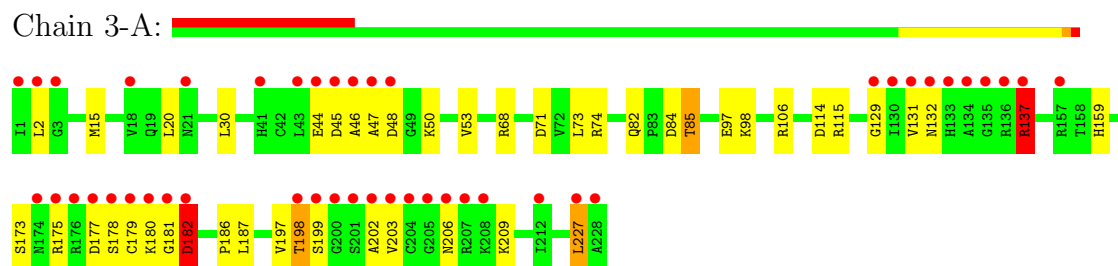
• Molecule 1: COMPLEMENT FACTOR D



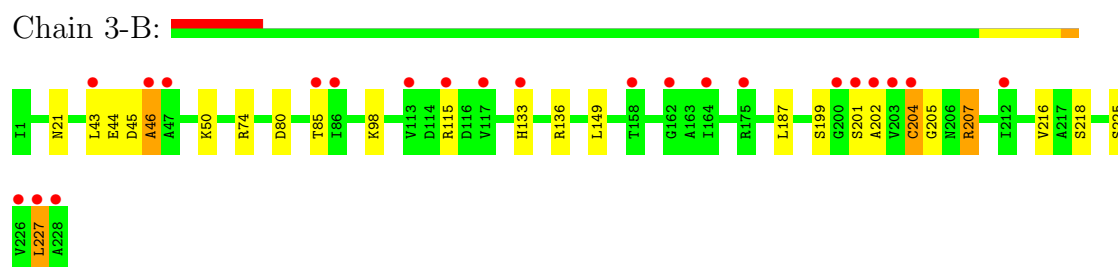
• Molecule 1: COMPLEMENT FACTOR D



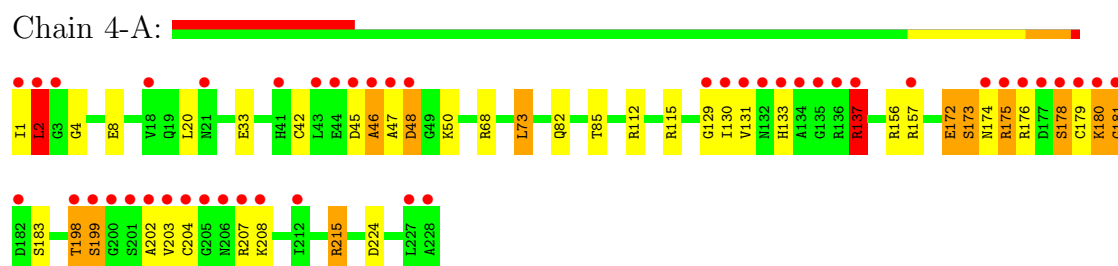
- Molecule 1: COMPLEMENT FACTOR D



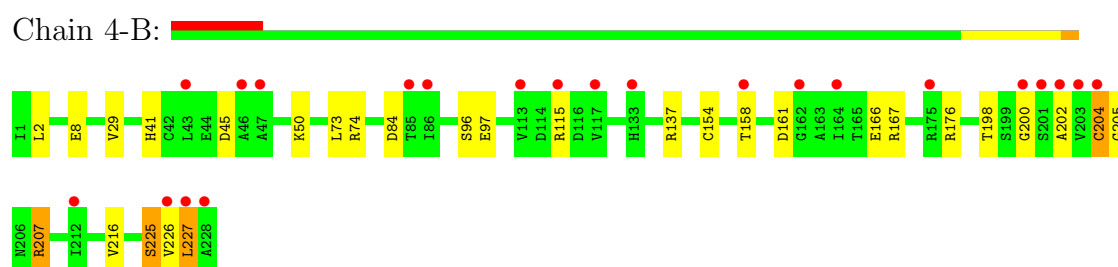
- Molecule 1: COMPLEMENT FACTOR D



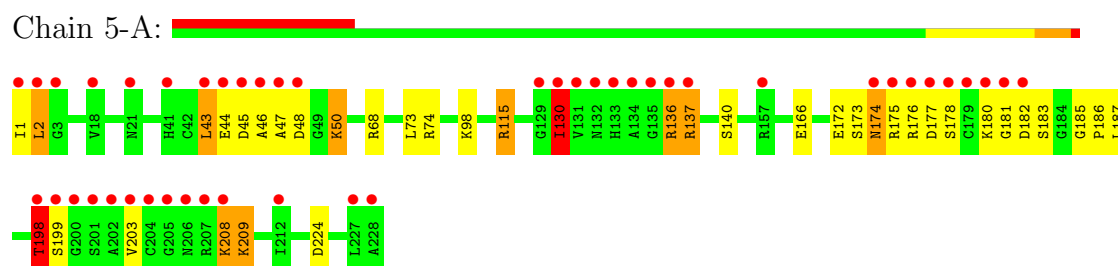
- Molecule 1: COMPLEMENT FACTOR D



- Molecule 1: COMPLEMENT FACTOR D

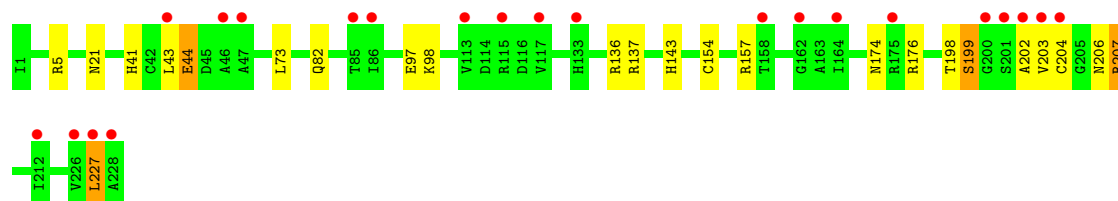


- Molecule 1: COMPLEMENT FACTOR D



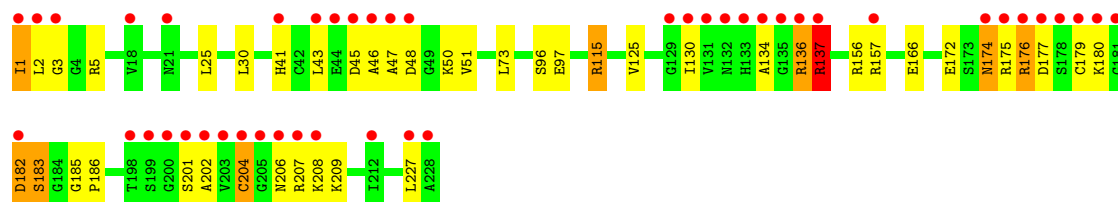
- Molecule 1: COMPLEMENT FACTOR D

Chain 5-B: 



- Molecule 1: COMPLEMENT FACTOR D

Chain 6-A: 



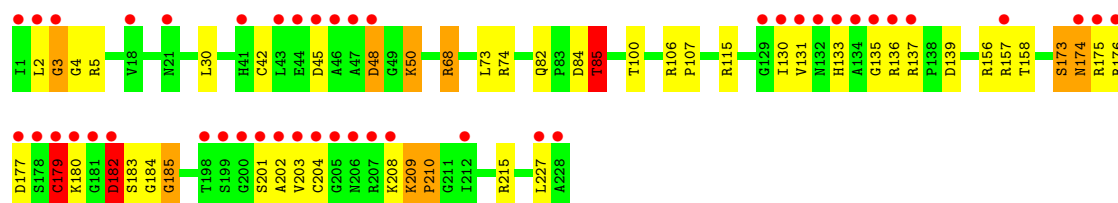
- Molecule 1: COMPLEMENT FACTOR D

Chain 6-B: 



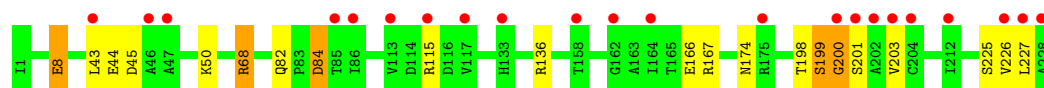
- Molecule 1: COMPLEMENT FACTOR D

Chain 7-A: 



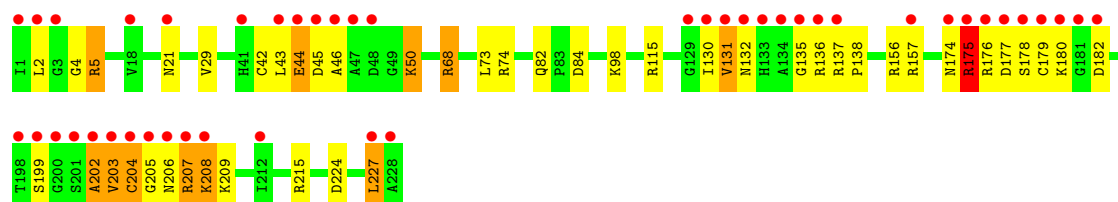
- Molecule 1: COMPLEMENT FACTOR D

Chain 7-B: 



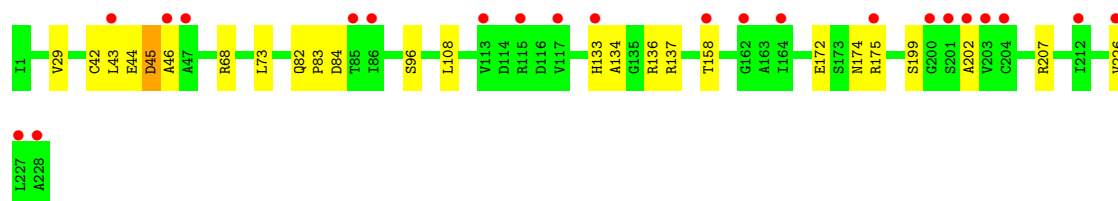
- Molecule 1: COMPLEMENT FACTOR D

Chain 8-A: 



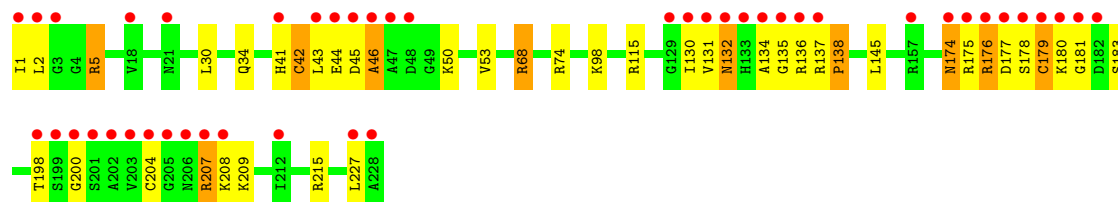
- Molecule 1: COMPLEMENT FACTOR D

Chain 8-B: 



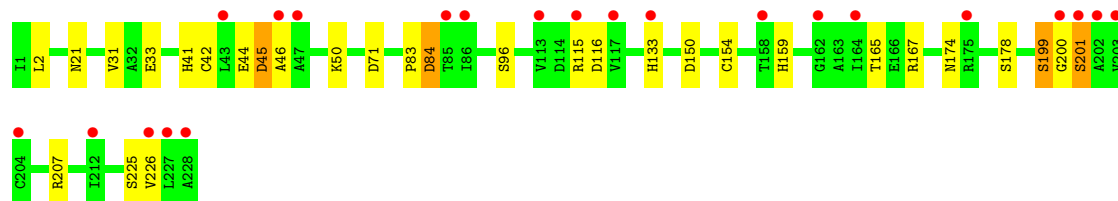
- Molecule 1: COMPLEMENT FACTOR D

Chain 9-A: 



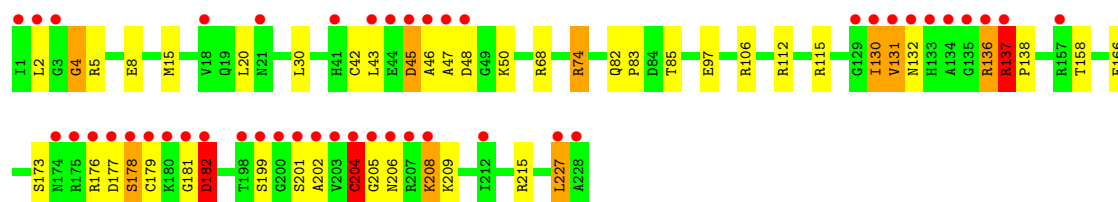
- Molecule 1: COMPLEMENT FACTOR D

Chain 9-B: 



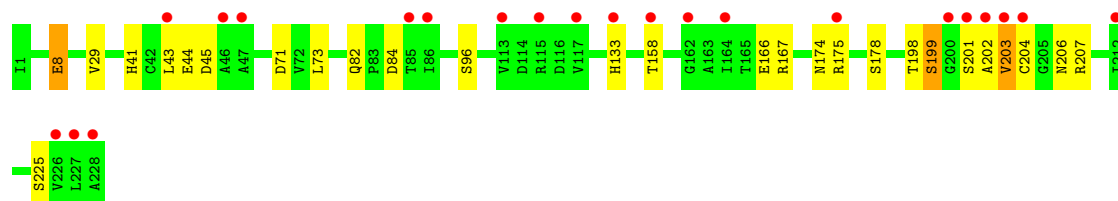
- Molecule 1: COMPLEMENT FACTOR D

Chain 10-A: 



- Molecule 1: COMPLEMENT FACTOR D

Chain 10-B: 



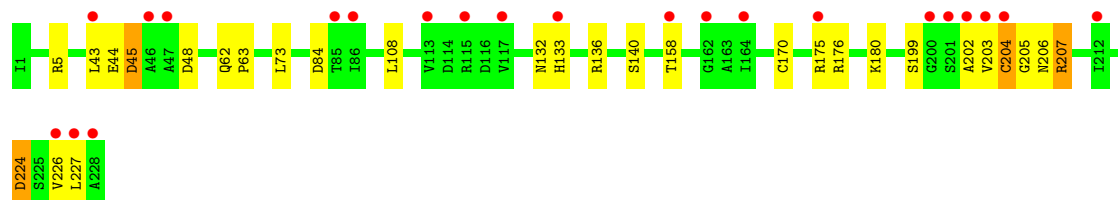
- Molecule 1: COMPLEMENT FACTOR D

Chain 11-A: 



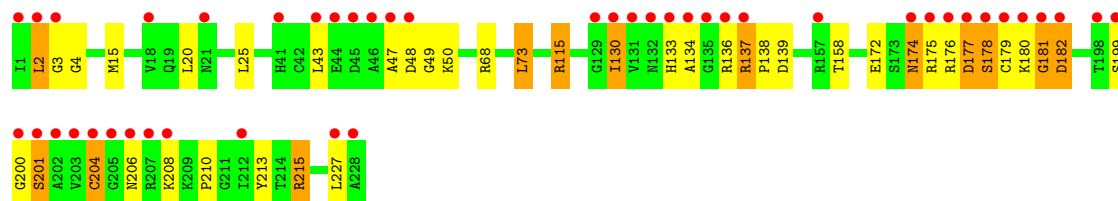
- Molecule 1: COMPLEMENT FACTOR D

Chain 11-B: 



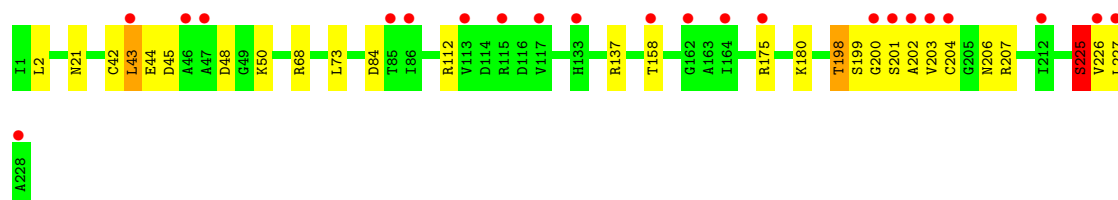
- Molecule 1: COMPLEMENT FACTOR D

Chain 12-A: 



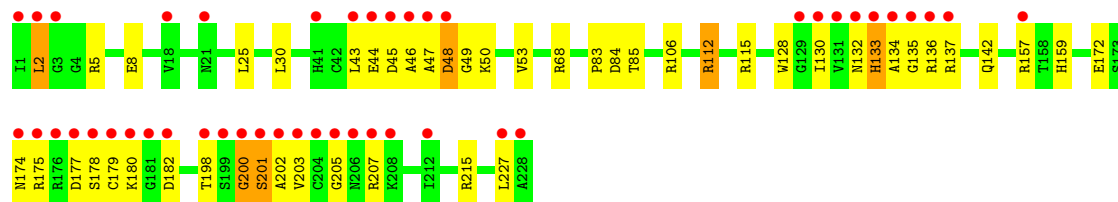
- Molecule 1: COMPLEMENT FACTOR D

Chain 12-B: 



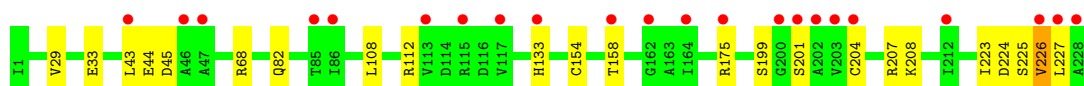
- Molecule 1: COMPLEMENT FACTOR D

Chain 13-A: 



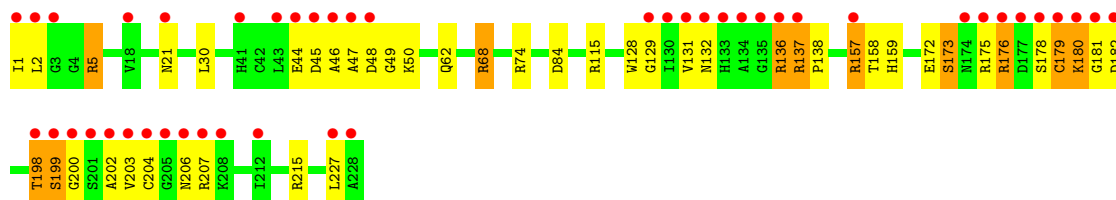
- Molecule 1: COMPLEMENT FACTOR D

Chain 13-B: 



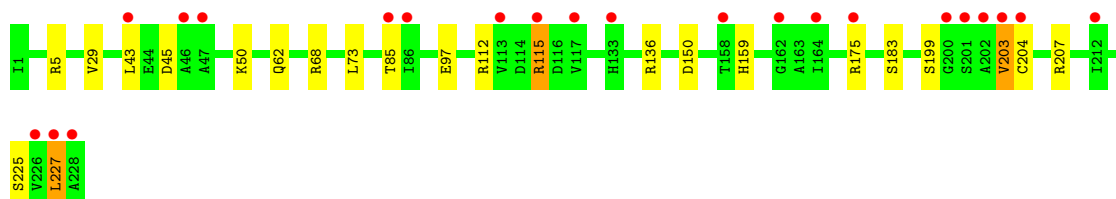
• Molecule 1: COMPLEMENT FACTOR D

Chain 14-A:



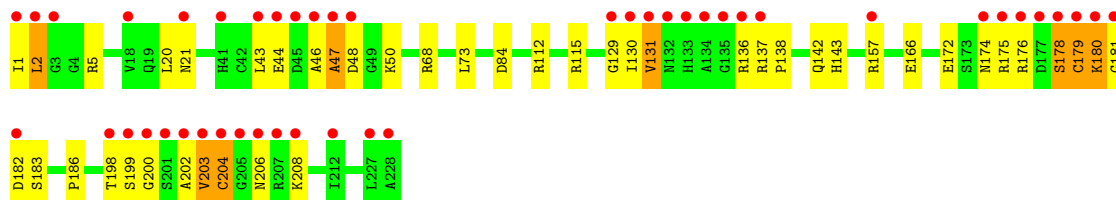
• Molecule 1: COMPLEMENT FACTOR D

Chain 14-B:



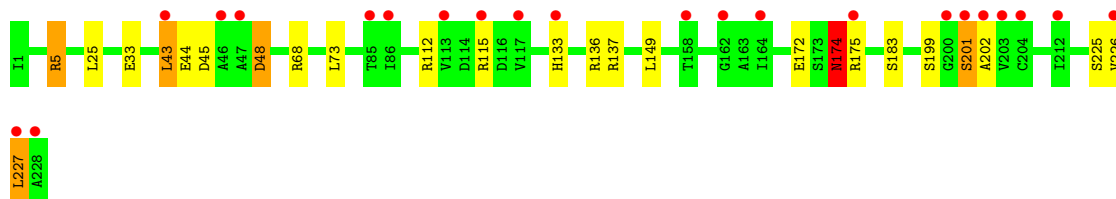
• Molecule 1: COMPLEMENT FACTOR D

Chain 15-A:



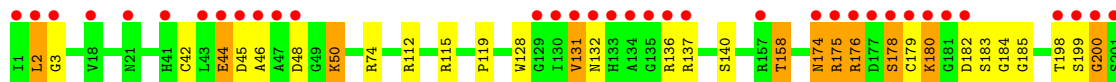
• Molecule 1: COMPLEMENT FACTOR D

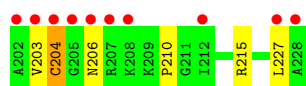
Chain 15-B:



• Molecule 1: COMPLEMENT FACTOR D

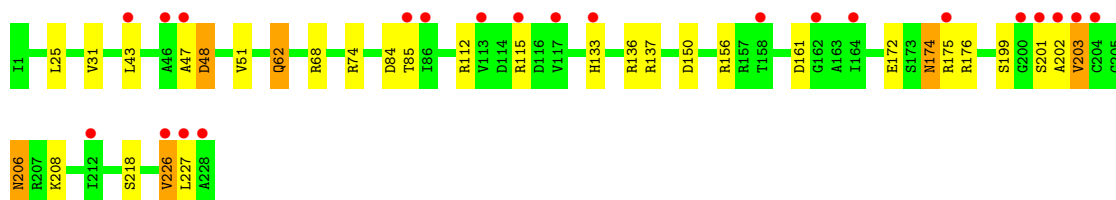
Chain 16-A:





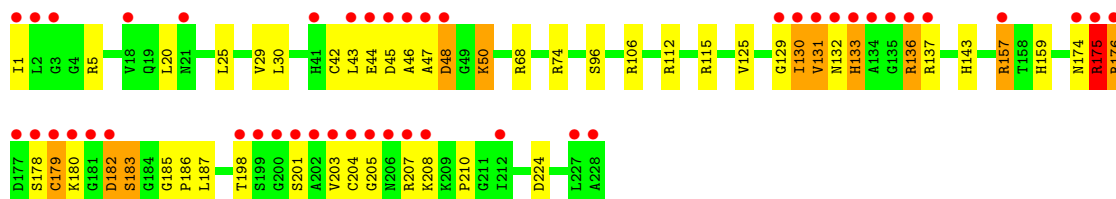
• Molecule 1: COMPLEMENT FACTOR D

Chain 16-B:



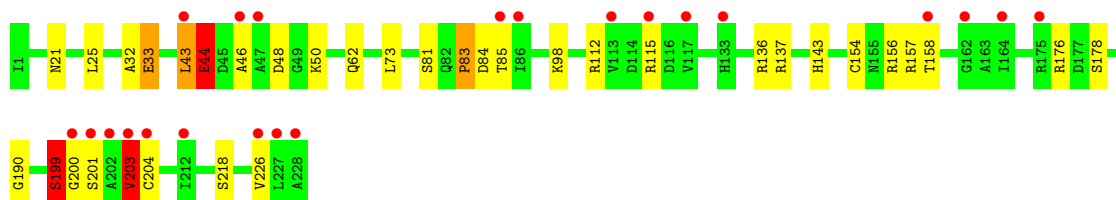
• Molecule 1: COMPLEMENT FACTOR D

Chain 17-A:



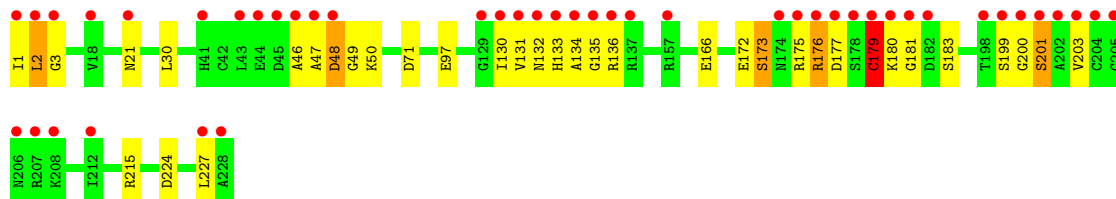
• Molecule 1: COMPLEMENT FACTOR D

Chain 17-B:



• Molecule 1: COMPLEMENT FACTOR D

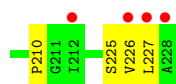
Chain 18-A:



• Molecule 1: COMPLEMENT FACTOR D

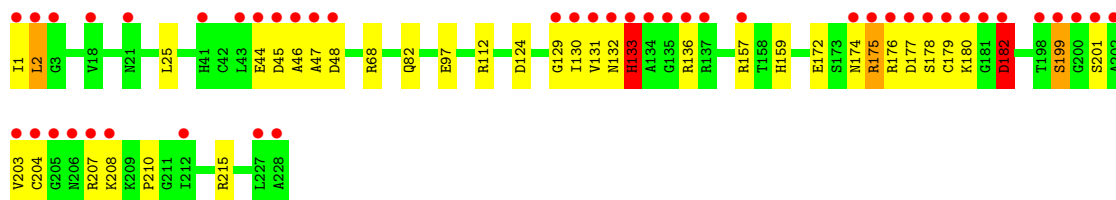
Chain 18-B:





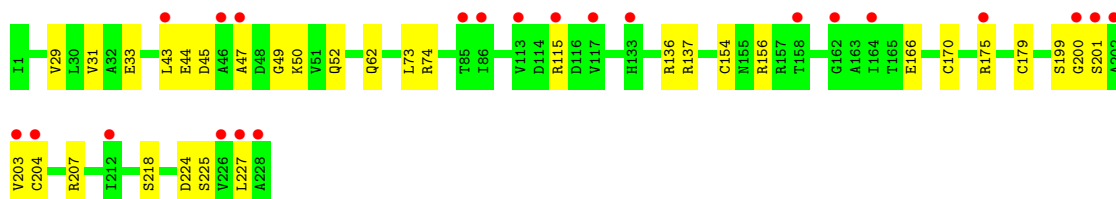
• Molecule 1: COMPLEMENT FACTOR D

Chain 19-A:



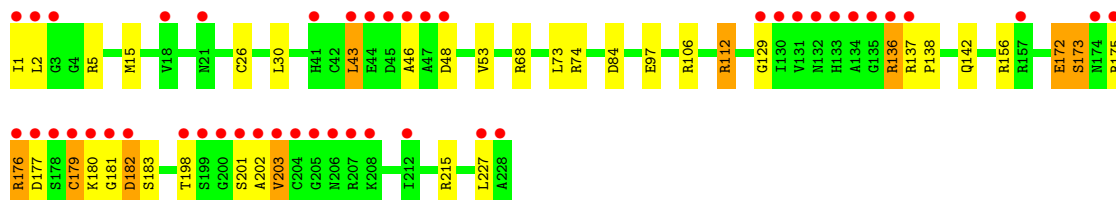
• Molecule 1: COMPLEMENT FACTOR D

Chain 19-B:



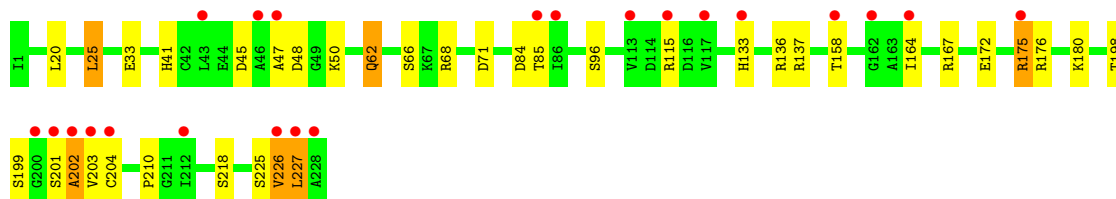
• Molecule 1: COMPLEMENT FACTOR D

Chain 20-A:



• Molecule 1: COMPLEMENT FACTOR D

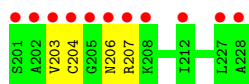
Chain 20-B:



• Molecule 1: COMPLEMENT FACTOR D

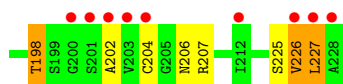
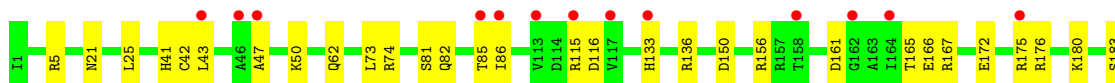
Chain 21-A:





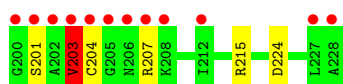
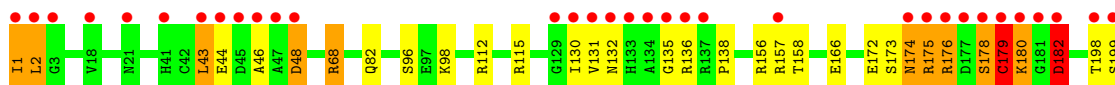
• Molecule 1: COMPLEMENT FACTOR D

Chain 21-B:



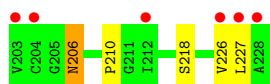
• Molecule 1: COMPLEMENT FACTOR D

Chain 22-A:



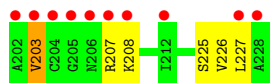
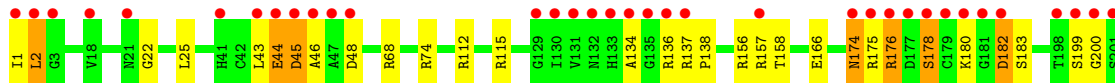
• Molecule 1: COMPLEMENT FACTOR D

Chain 22-B:



• Molecule 1: COMPLEMENT FACTOR D

Chain 23-A:



• Molecule 1: COMPLEMENT FACTOR D

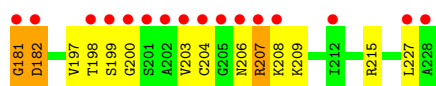
Chain 23-B:





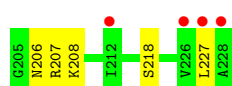
• Molecule 1: COMPLEMENT FACTOR D

Chain 24-A:



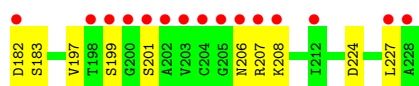
• Molecule 1: COMPLEMENT FACTOR D

Chain 24-B:



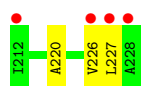
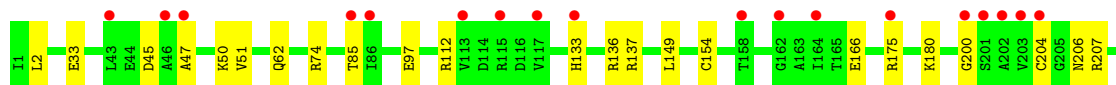
• Molecule 1: COMPLEMENT FACTOR D

Chain 25-A:



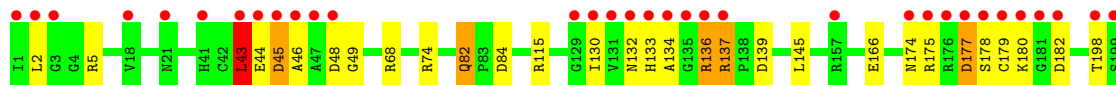
• Molecule 1: COMPLEMENT FACTOR D

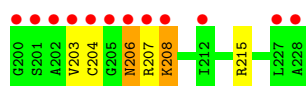
Chain 25-B:



• Molecule 1: COMPLEMENT FACTOR D

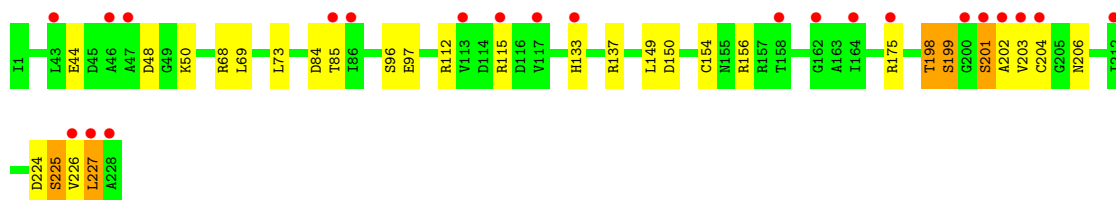
Chain 26-A:





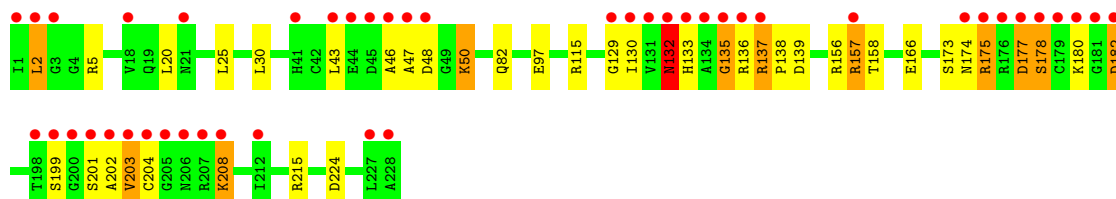
• Molecule 1: COMPLEMENT FACTOR D

Chain 26-B:



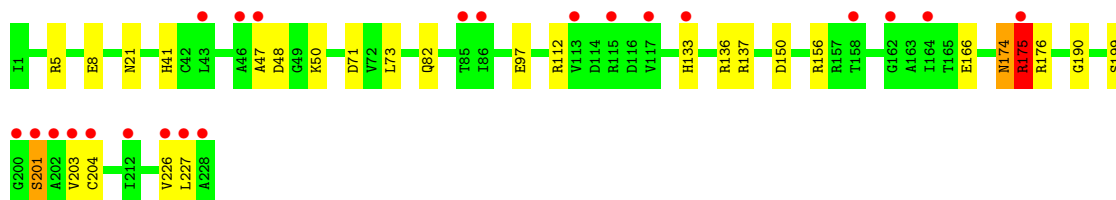
• Molecule 1: COMPLEMENT FACTOR D

Chain 27-A:



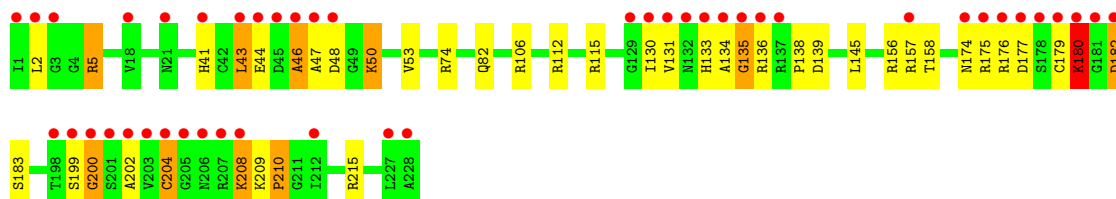
• Molecule 1: COMPLEMENT FACTOR D

Chain 27-B:



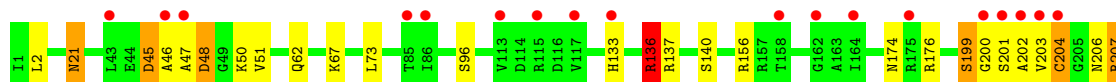
• Molecule 1: COMPLEMENT FACTOR D

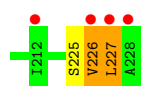
Chain 28-A:



• Molecule 1: COMPLEMENT FACTOR D

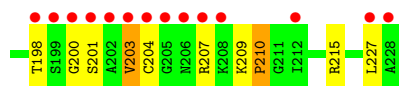
Chain 28-B:





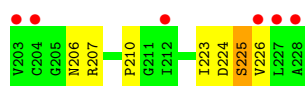
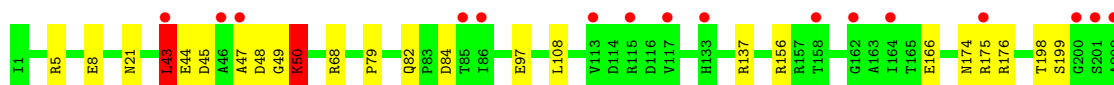
• Molecule 1: COMPLEMENT FACTOR D

Chain 29-A:



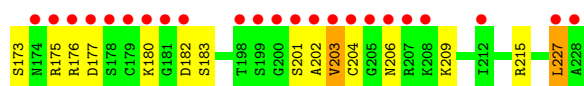
• Molecule 1: COMPLEMENT FACTOR D

Chain 29-B:



• Molecule 1: COMPLEMENT FACTOR D

Chain 30-A:



• Molecule 1: COMPLEMENT FACTOR D

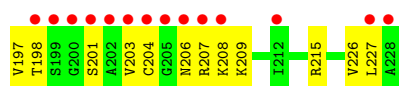
Chain 30-B:



• Molecule 1: COMPLEMENT FACTOR D

Chain 31-A:





- Molecule 1: COMPLEMENT FACTOR D

Chain 31-B:



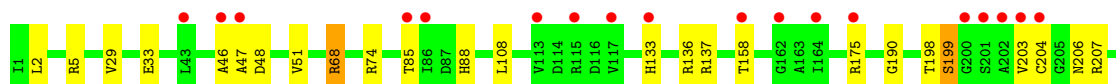
- Molecule 1: COMPLEMENT FACTOR D

Chain 32-A:



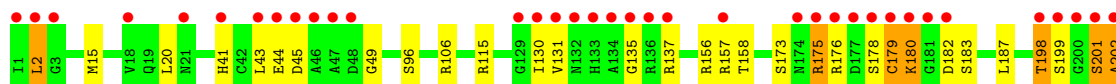
- Molecule 1: COMPLEMENT FACTOR D

Chain 32-B:



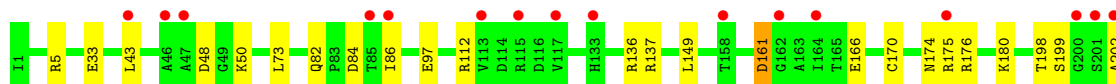
- Molecule 1: COMPLEMENT FACTOR D

Chain 33-A:

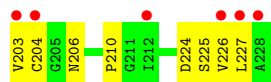


- Molecule 1: COMPLEMENT FACTOR D

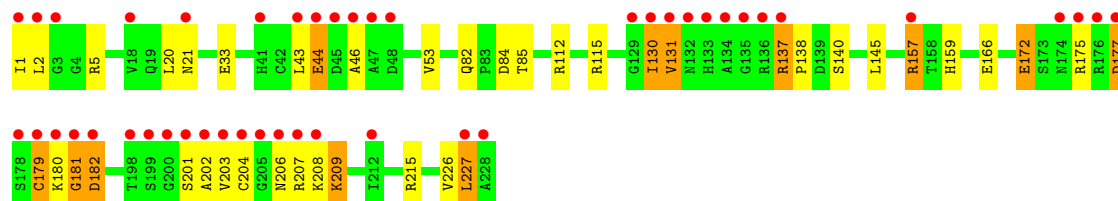
Chain 33-B:



- Molecule 1: COMPLEMENT FACTOR D

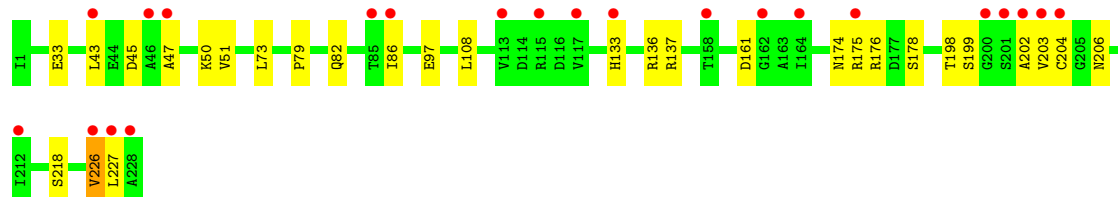


Chain 34-A:



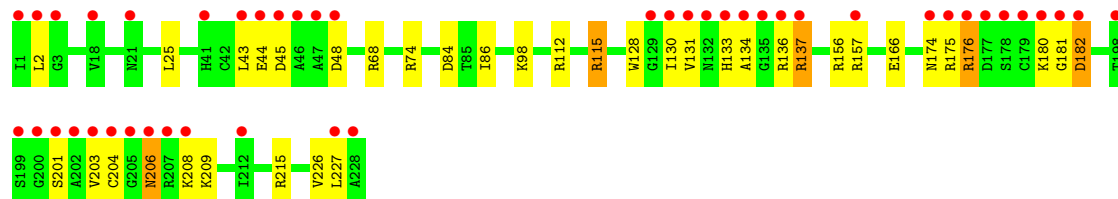
• Molecule 1: COMPLEMENT FACTOR D

Chain 34-B:



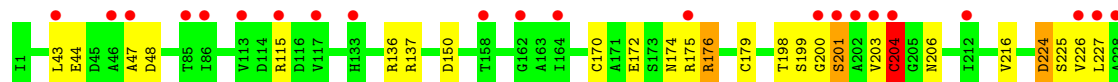
• Molecule 1: COMPLEMENT FACTOR D

Chain 35-A:



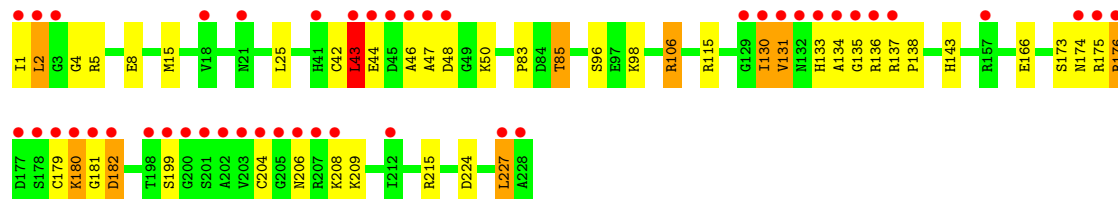
• Molecule 1: COMPLEMENT FACTOR D

Chain 35-B:



• Molecule 1: COMPLEMENT FACTOR D

Chain 36-A:



• Molecule 1: COMPLEMENT FACTOR D

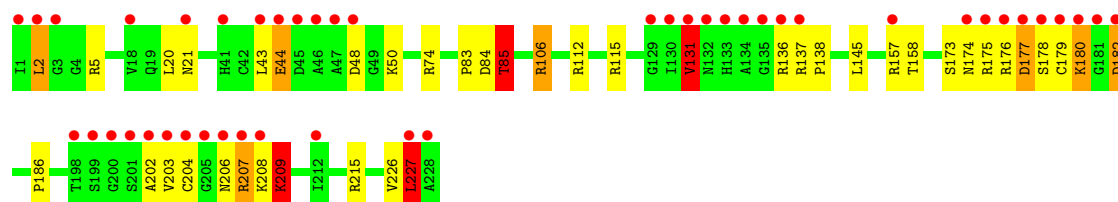
Chain 36-B:





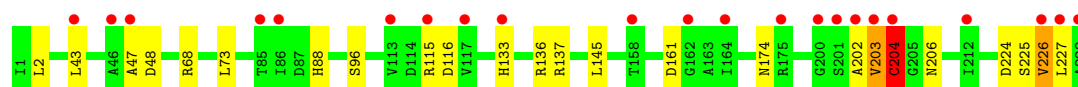
• Molecule 1: COMPLEMENT FACTOR D

Chain 37-A:



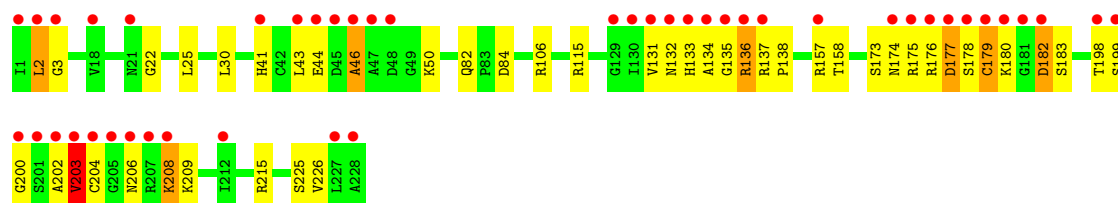
• Molecule 1: COMPLEMENT FACTOR D

Chain 37-B:



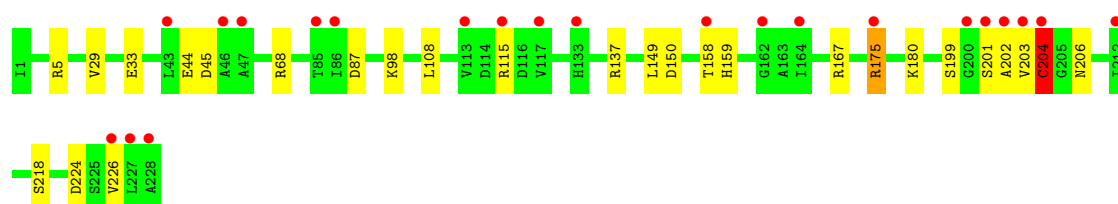
• Molecule 1: COMPLEMENT FACTOR D

Chain 38-A:



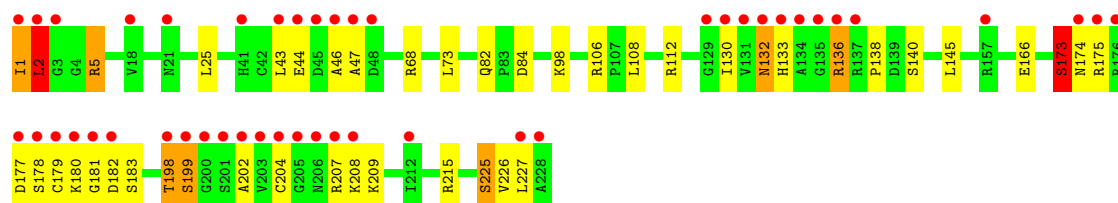
• Molecule 1: COMPLEMENT FACTOR D

Chain 38-B:

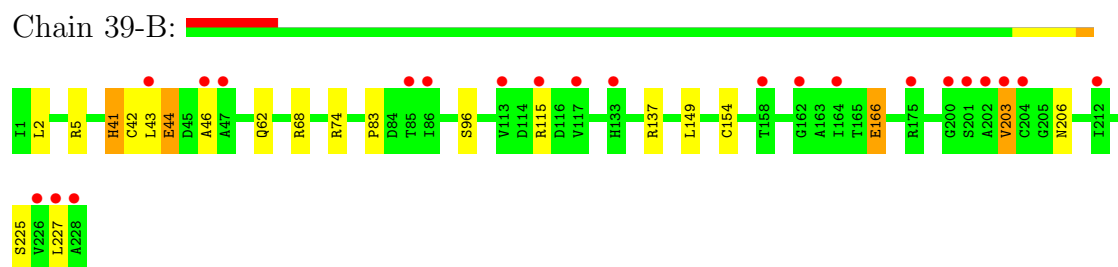


• Molecule 1: COMPLEMENT FACTOR D

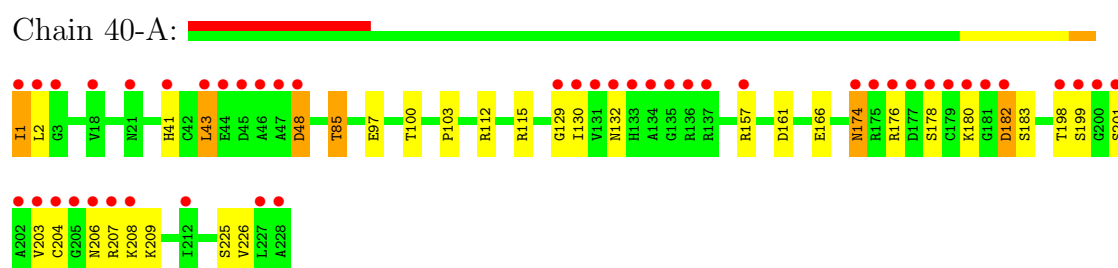
Chain 39-A:



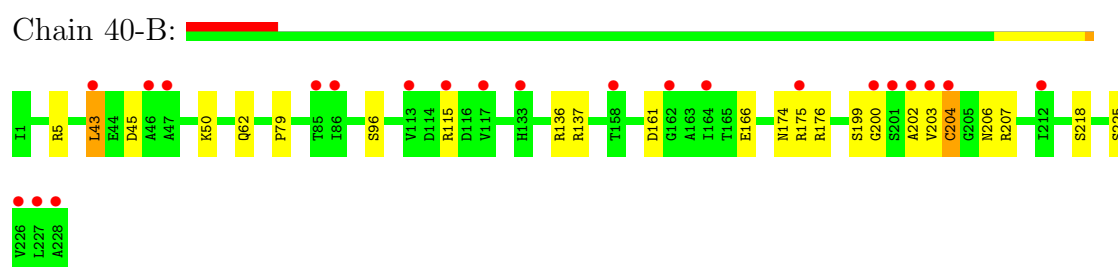
• Molecule 1: COMPLEMENT FACTOR D



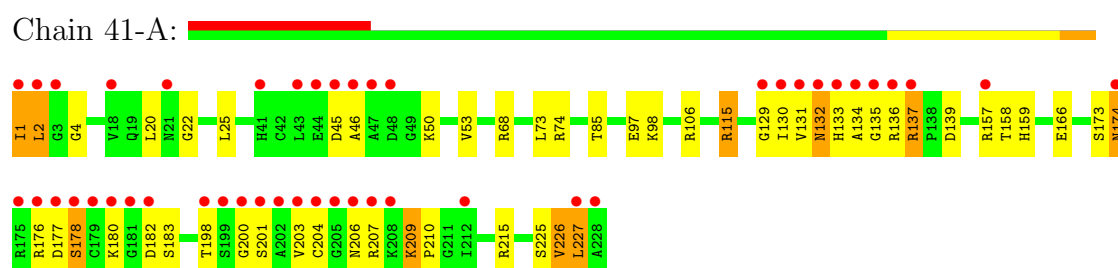
- Molecule 1: COMPLEMENT FACTOR D



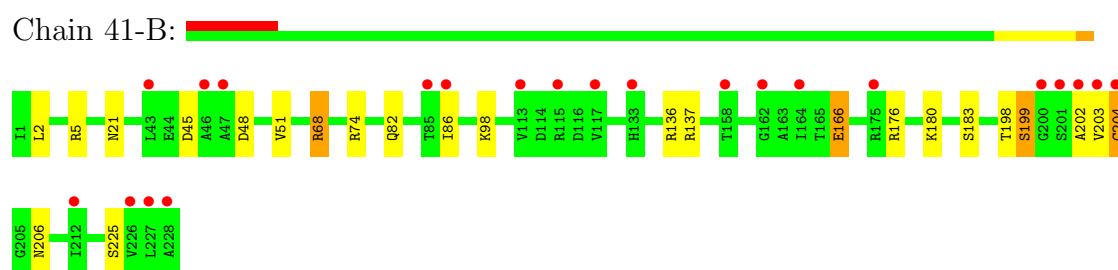
- Molecule 1: COMPLEMENT FACTOR D



- Molecule 1: COMPLEMENT FACTOR D

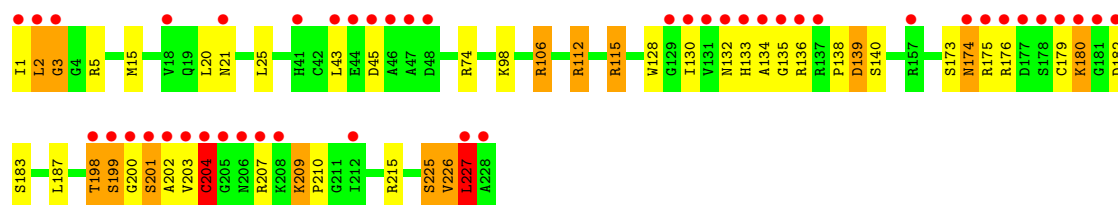


- Molecule 1: COMPLEMENT FACTOR D



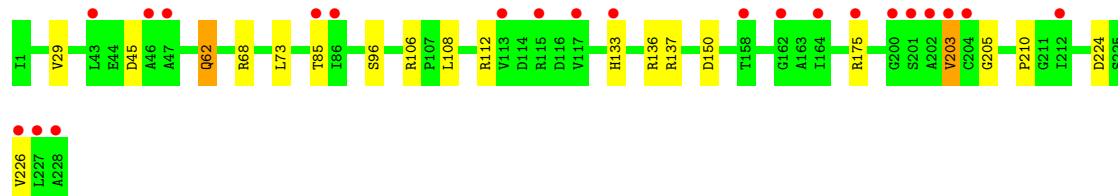
- Molecule 1: COMPLEMENT FACTOR D





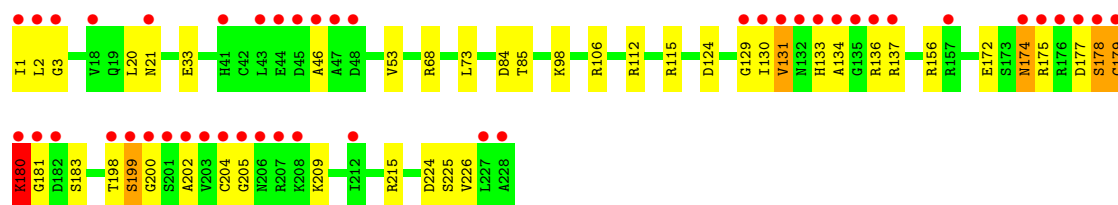
• Molecule 1: COMPLEMENT FACTOR D

Chain 42-B:



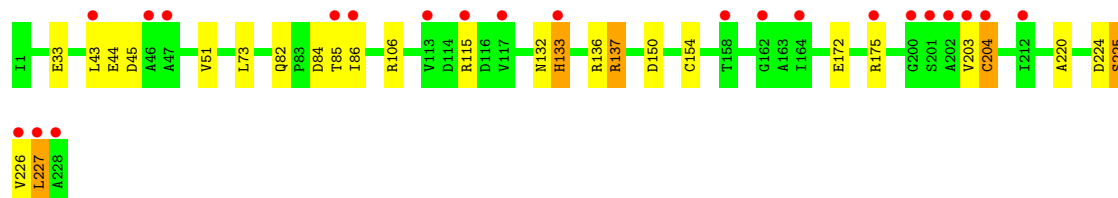
• Molecule 1: COMPLEMENT FACTOR D

Chain 43-A:



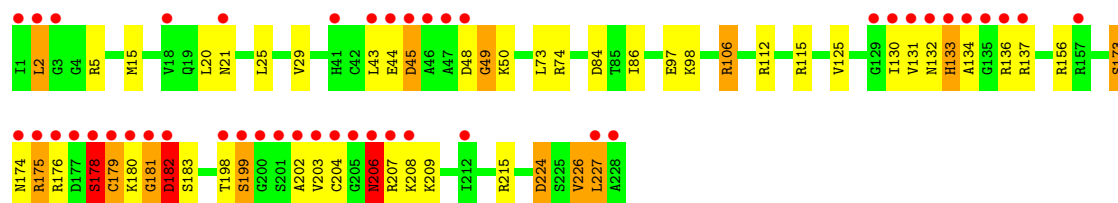
• Molecule 1: COMPLEMENT FACTOR D

Chain 43-B:



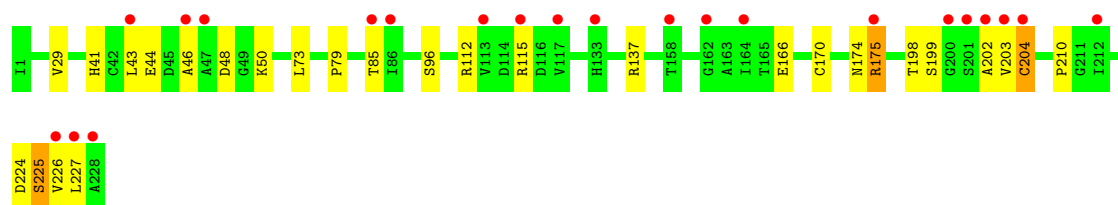
• Molecule 1: COMPLEMENT FACTOR D

Chain 44-A:



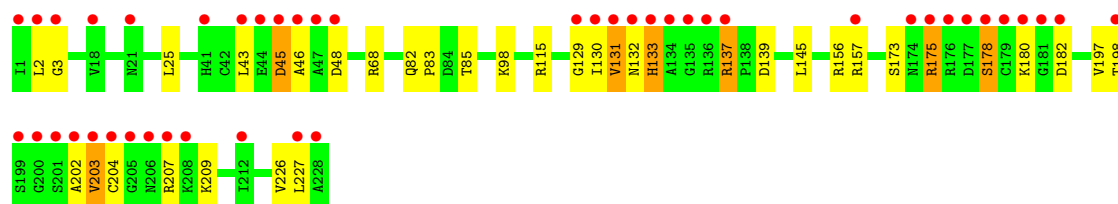
• Molecule 1: COMPLEMENT FACTOR D

Chain 44-B:



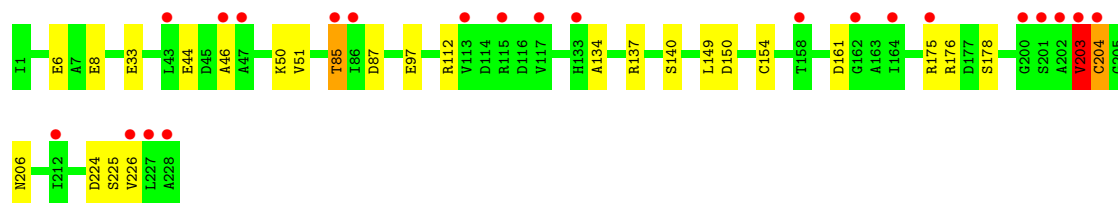
• Molecule 1: COMPLEMENT FACTOR D

Chain 45-A:



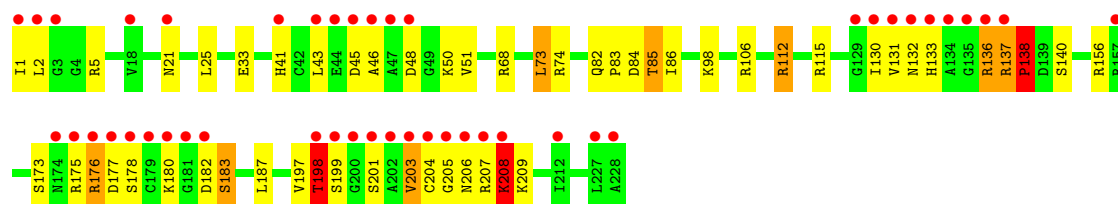
• Molecule 1: COMPLEMENT FACTOR D

Chain 45-B:



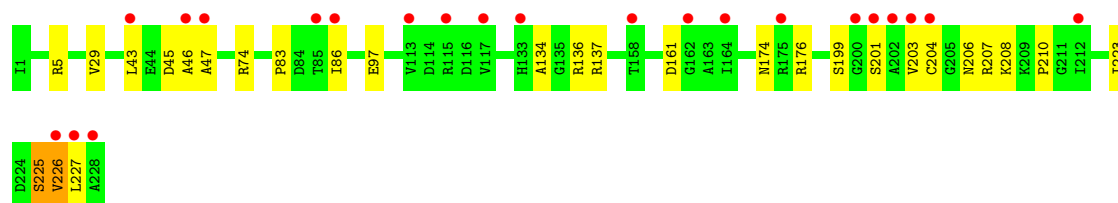
• Molecule 1: COMPLEMENT FACTOR D

Chain 46-A:



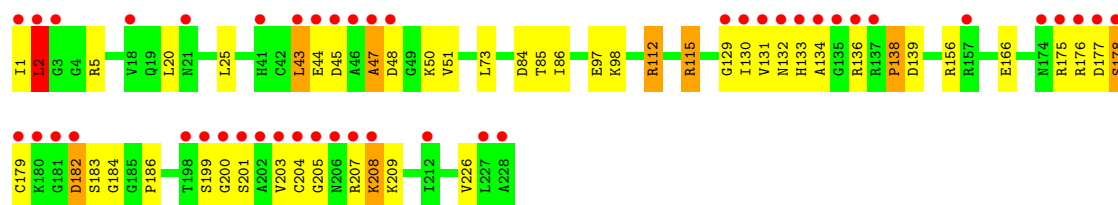
• Molecule 1: COMPLEMENT FACTOR D

Chain 46-B:



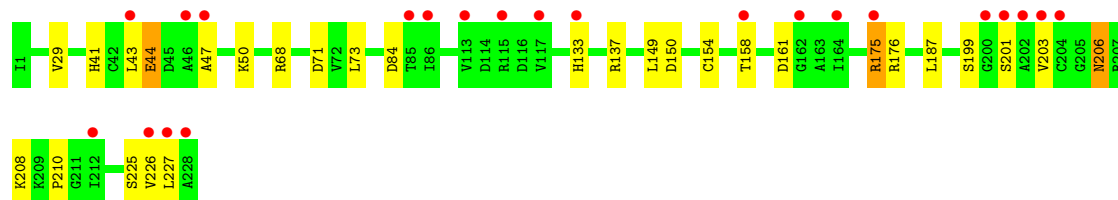
• Molecule 1: COMPLEMENT FACTOR D

Chain 47-A:



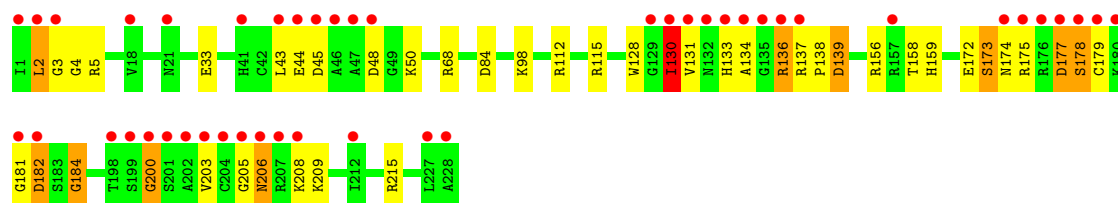
• Molecule 1: COMPLEMENT FACTOR D

Chain 47-B: 



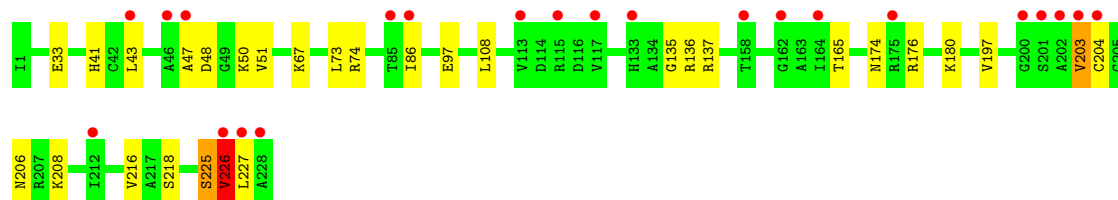
• Molecule 1: COMPLEMENT FACTOR D

Chain 48-A: 



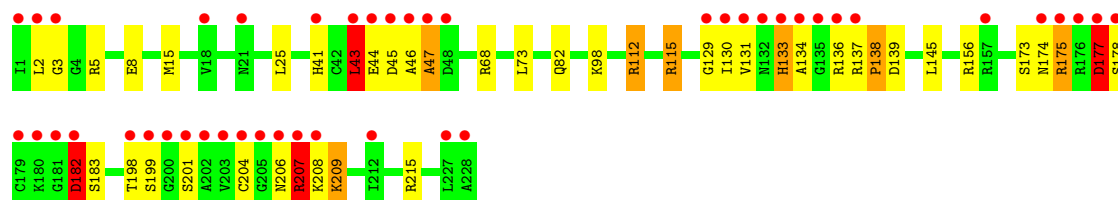
• Molecule 1: COMPLEMENT FACTOR D

Chain 48-B: 



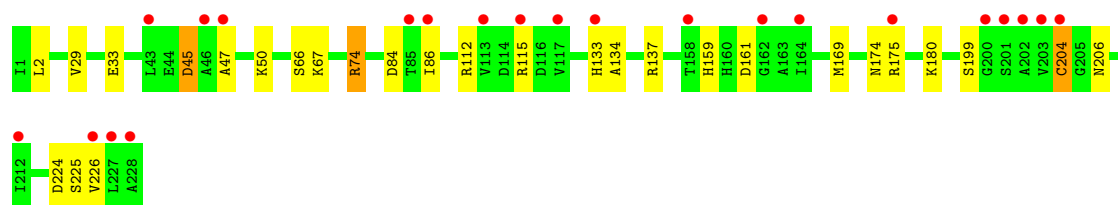
• Molecule 1: COMPLEMENT FACTOR D

Chain 49-A: 



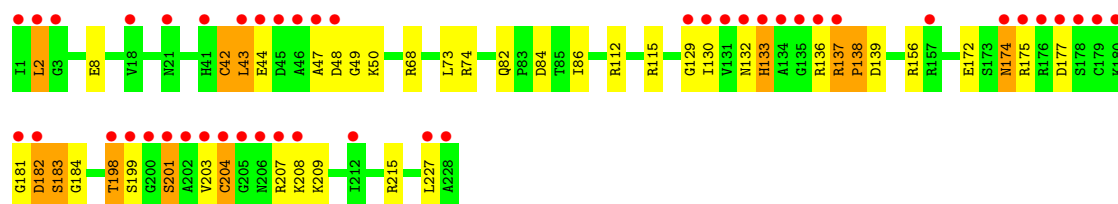
• Molecule 1: COMPLEMENT FACTOR D

Chain 49-B: 



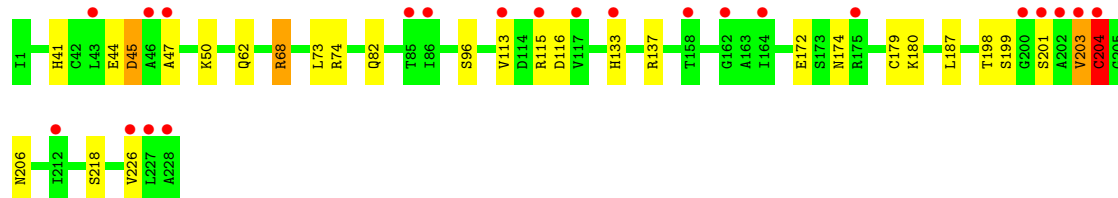
• Molecule 1: COMPLEMENT FACTOR D

Chain 50-A:



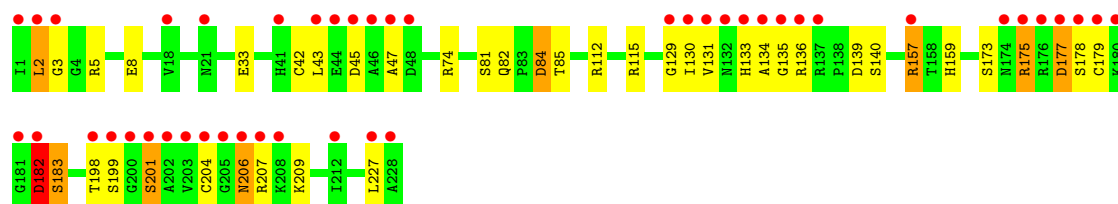
• Molecule 1: COMPLEMENT FACTOR D

Chain 50-B:



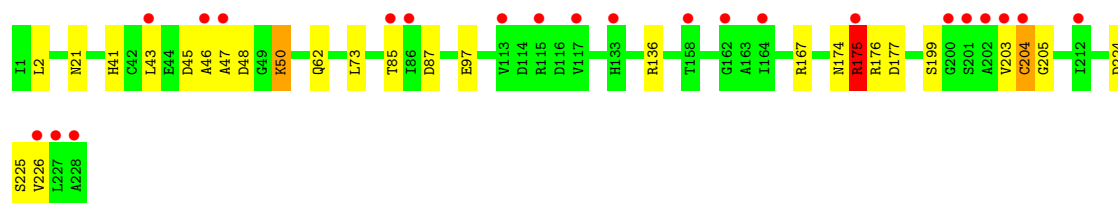
• Molecule 1: COMPLEMENT FACTOR D

Chain 51-A:



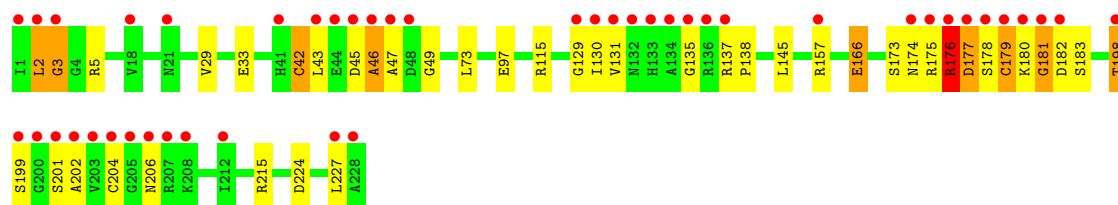
• Molecule 1: COMPLEMENT FACTOR D

Chain 51-B:



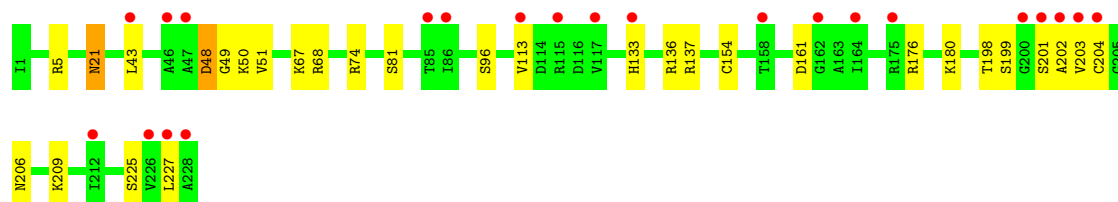
• Molecule 1: COMPLEMENT FACTOR D

Chain 52-A:



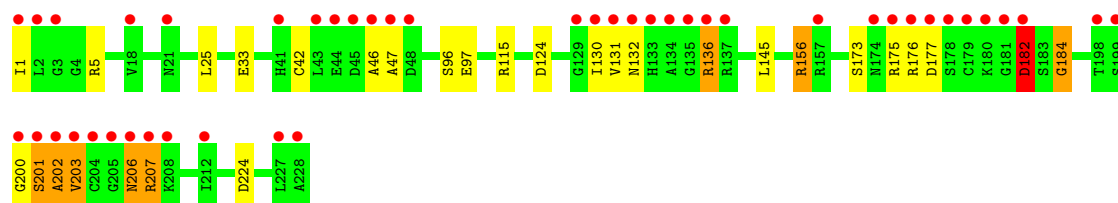
• Molecule 1: COMPLEMENT FACTOR D

Chain 52-B:



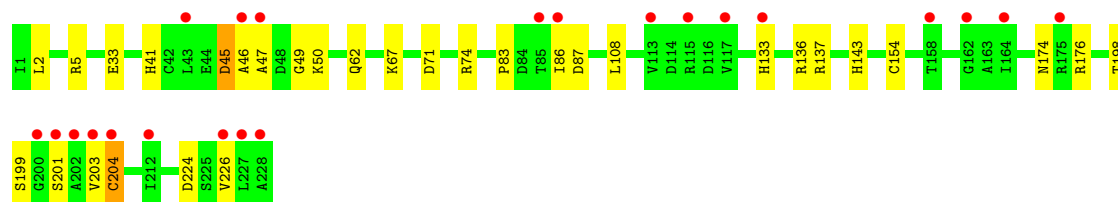
• Molecule 1: COMPLEMENT FACTOR D

Chain 53-A:



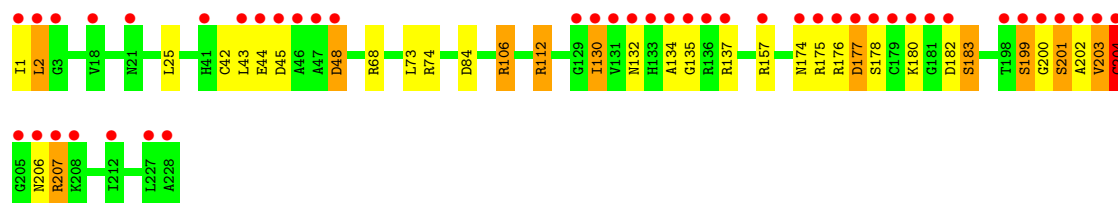
• Molecule 1: COMPLEMENT FACTOR D

Chain 53-B:



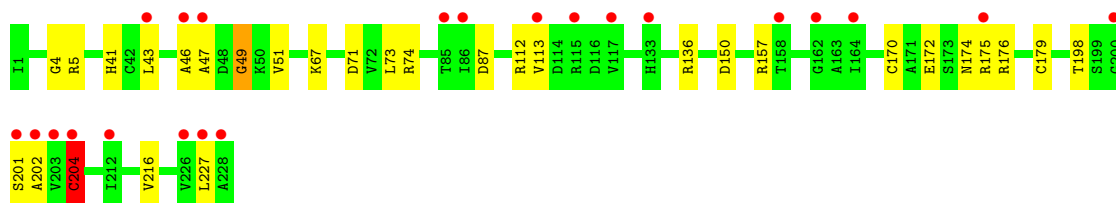
• Molecule 1: COMPLEMENT FACTOR D

Chain 54-A:



• Molecule 1: COMPLEMENT FACTOR D

Chain 54-B:



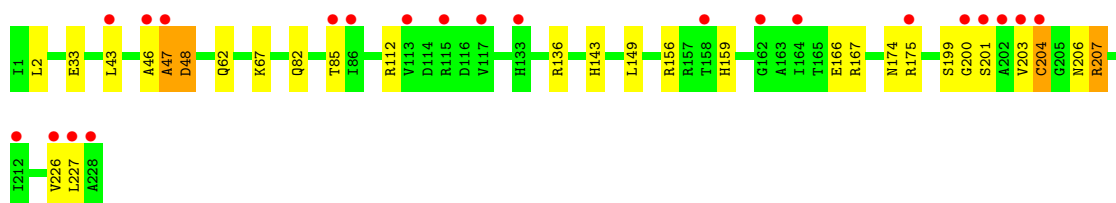
- Molecule 1: COMPLEMENT FACTOR D

Chain 55-A:



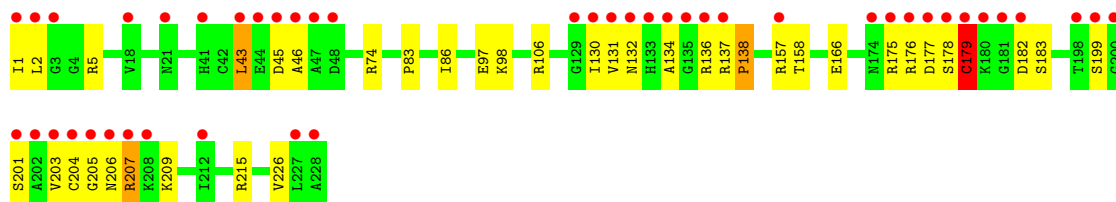
- Molecule 1: COMPLEMENT FACTOR D

Chain 55-B:



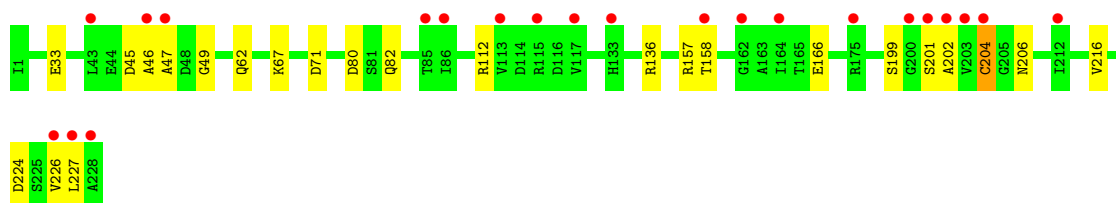
- Molecule 1: COMPLEMENT FACTOR D

Chain 56-A:



- Molecule 1: COMPLEMENT FACTOR D

Chain 56-B:



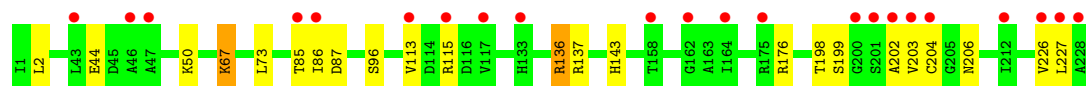
- Molecule 1: COMPLEMENT FACTOR D

Chain 57-A:



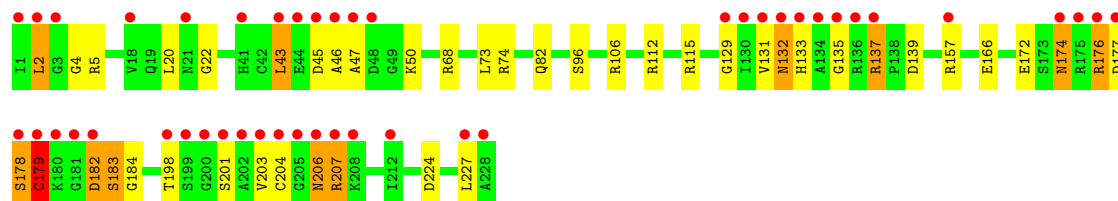
• Molecule 1: COMPLEMENT FACTOR D

Chain 57-B:



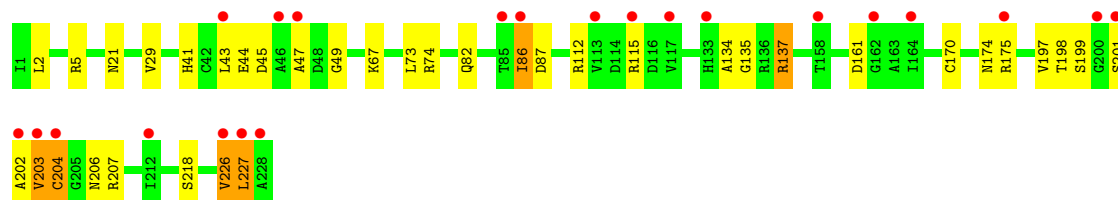
• Molecule 1: COMPLEMENT FACTOR D

Chain 58-A:



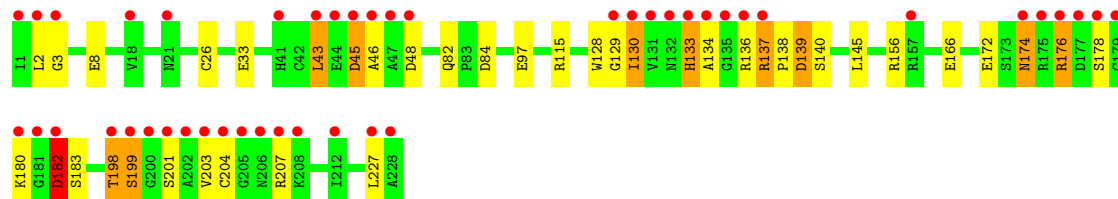
• Molecule 1: COMPLEMENT FACTOR D

Chain 58-B:



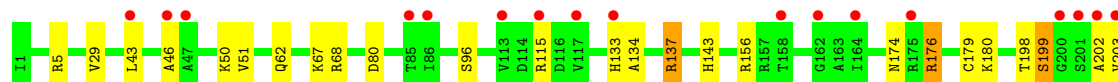
• Molecule 1: COMPLEMENT FACTOR D

Chain 59-A:



• Molecule 1: COMPLEMENT FACTOR D

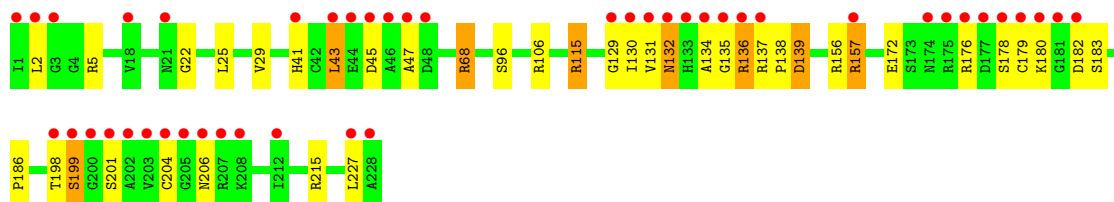
Chain 59-B:





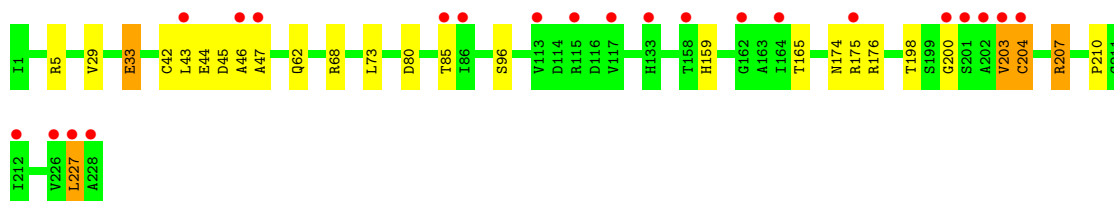
• Molecule 1: COMPLEMENT FACTOR D

Chain 60-A:



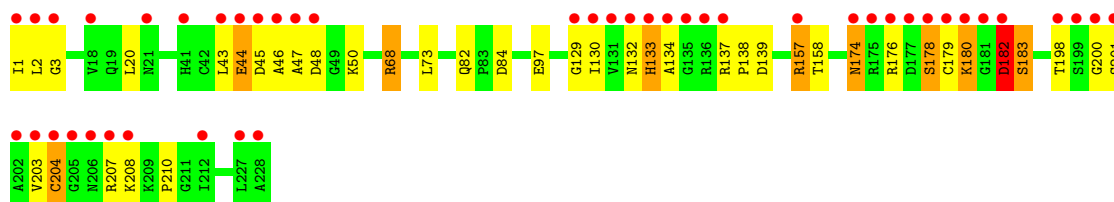
• Molecule 1: COMPLEMENT FACTOR D

Chain 60-B:



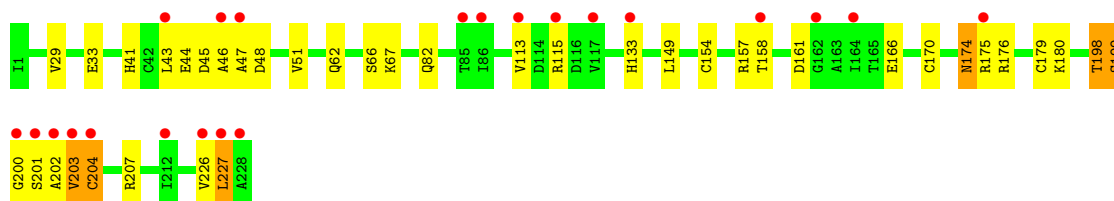
• Molecule 1: COMPLEMENT FACTOR D

Chain 61-A:



• Molecule 1: COMPLEMENT FACTOR D

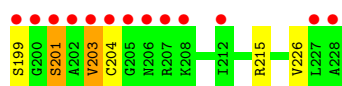
Chain 61-B:



• Molecule 1: COMPLEMENT FACTOR D

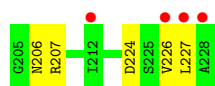
Chain 62-A:





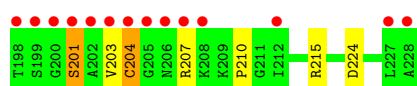
- Molecule 1: COMPLEMENT FACTOR D

Chain 62-B:



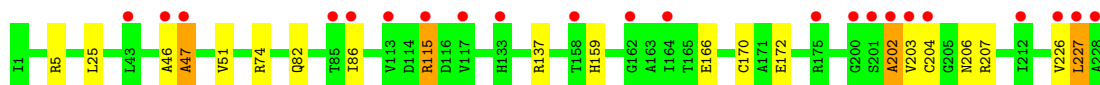
- Molecule 1: COMPLEMENT FACTOR D

Chain 63-A:



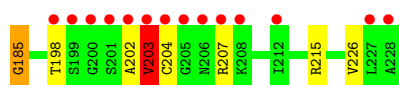
- Molecule 1: COMPLEMENT FACTOR D

Chain 63-B:



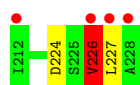
- Molecule 1: COMPLEMENT FACTOR D

Chain 64-A:



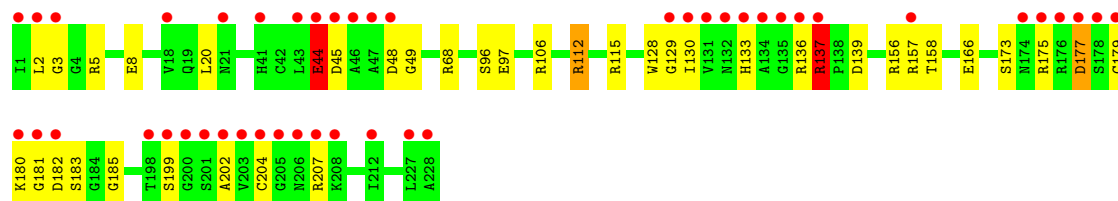
- Molecule 1: COMPLEMENT FACTOR D

Chain 64-B:



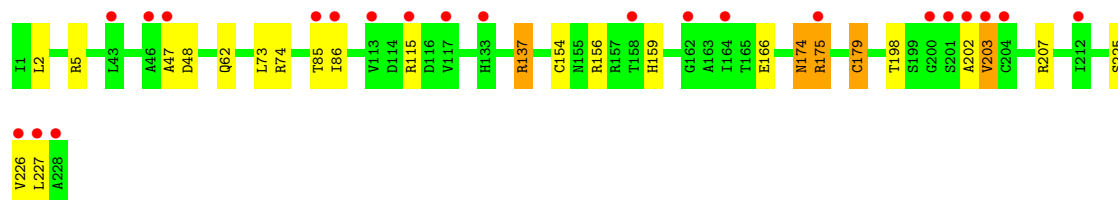
- Molecule 1: COMPLEMENT FACTOR D

Chain 65-A: 



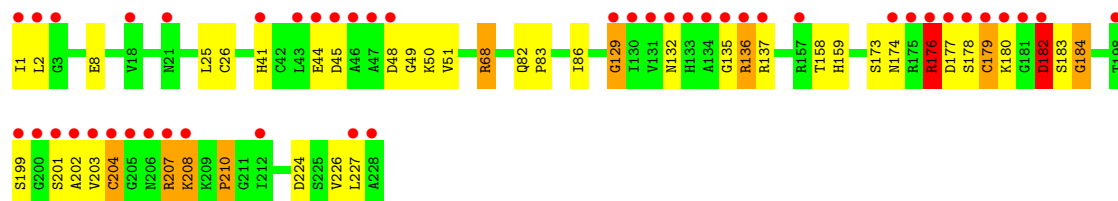
• Molecule 1: COMPLEMENT FACTOR D

Chain 65-B: 



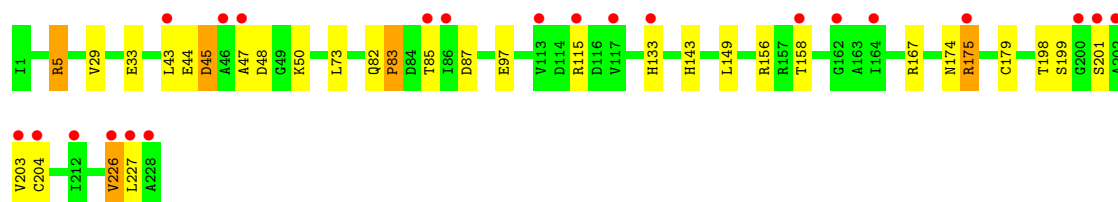
• Molecule 1: COMPLEMENT FACTOR D

Chain 66-A: 



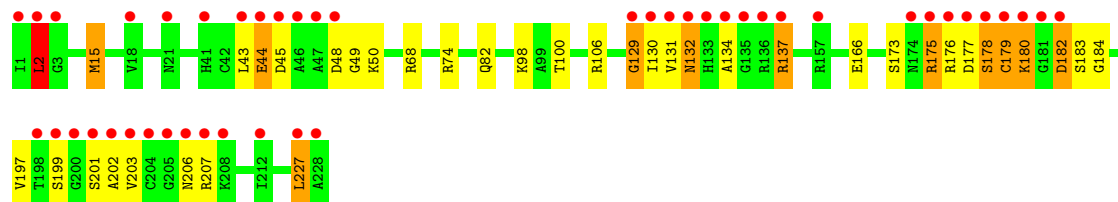
• Molecule 1: COMPLEMENT FACTOR D

Chain 66-B: 



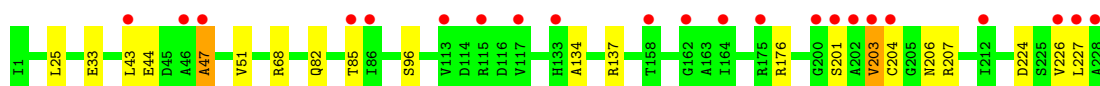
• Molecule 1: COMPLEMENT FACTOR D

Chain 67-A: 



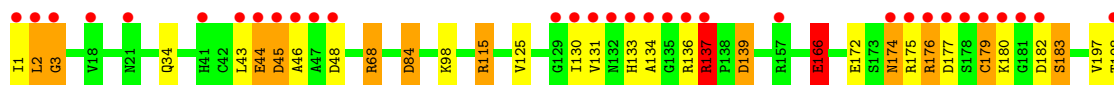
• Molecule 1: COMPLEMENT FACTOR D

Chain 67-B: 



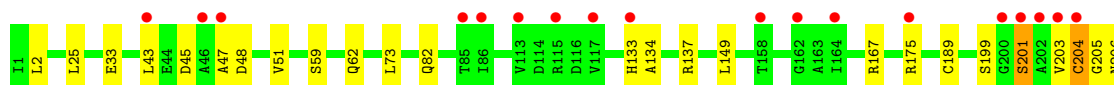
• Molecule 1: COMPLEMENT FACTOR D

Chain 68-A:



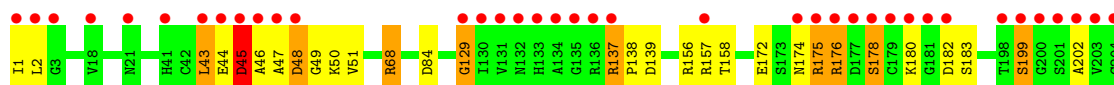
• Molecule 1: COMPLEMENT FACTOR D

Chain 68-B:



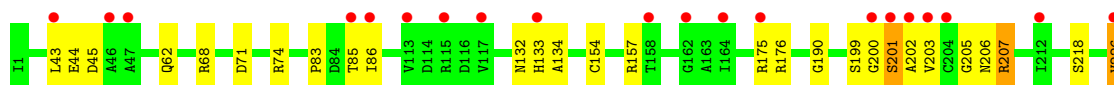
• Molecule 1: COMPLEMENT FACTOR D

Chain 69-A:



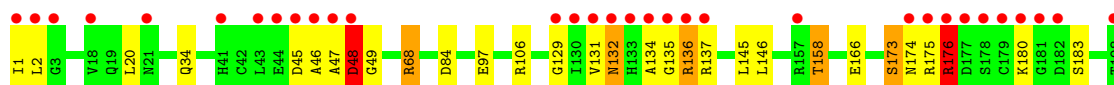
• Molecule 1: COMPLEMENT FACTOR D

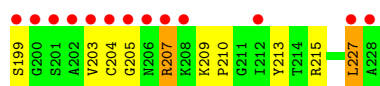
Chain 69-B:



• Molecule 1: COMPLEMENT FACTOR D

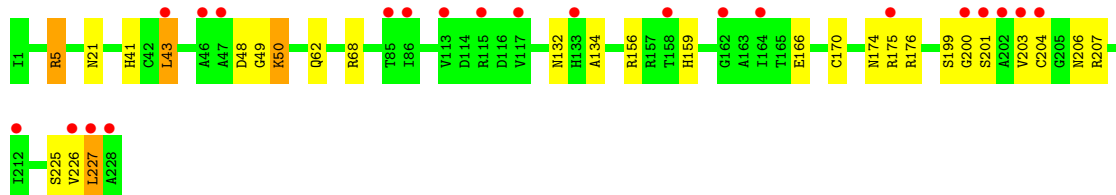
Chain 70-A:





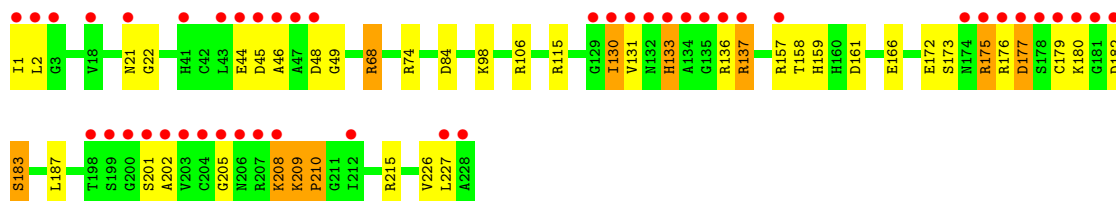
• Molecule 1: COMPLEMENT FACTOR D

Chain 70-B:



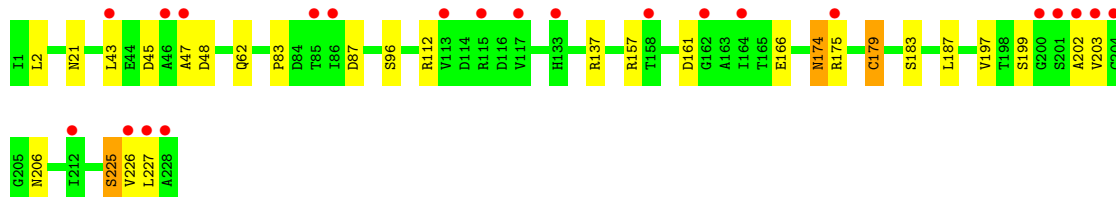
• Molecule 1: COMPLEMENT FACTOR D

Chain 71-A:



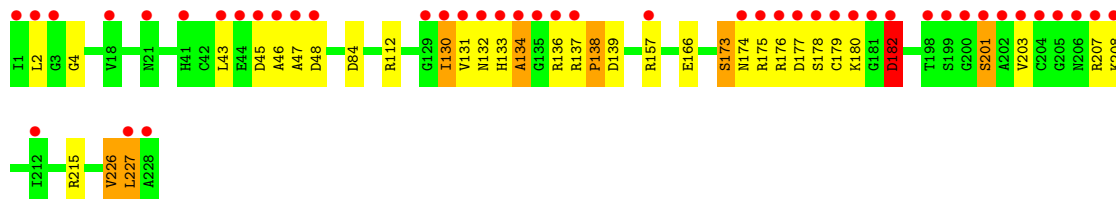
• Molecule 1: COMPLEMENT FACTOR D

Chain 71-B:



• Molecule 1: COMPLEMENT FACTOR D

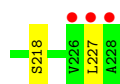
Chain 72-A:



• Molecule 1: COMPLEMENT FACTOR D

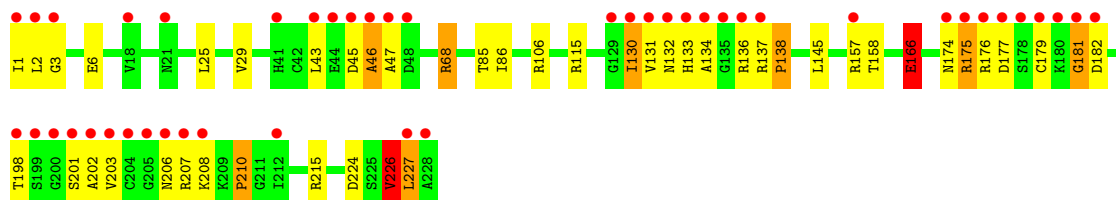
Chain 72-B:





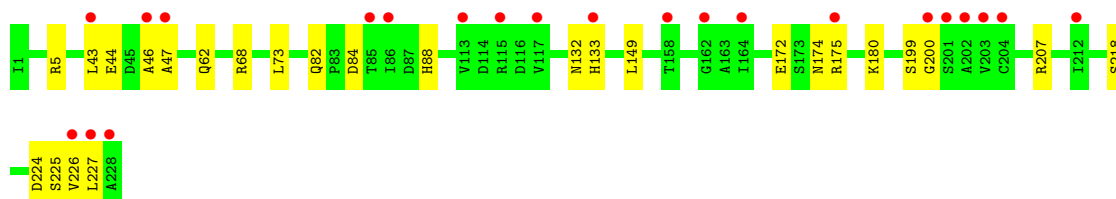
• Molecule 1: COMPLEMENT FACTOR D

Chain 73-A:



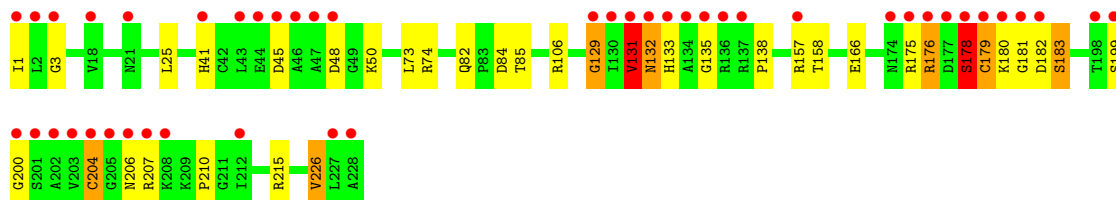
• Molecule 1: COMPLEMENT FACTOR D

Chain 73-B:



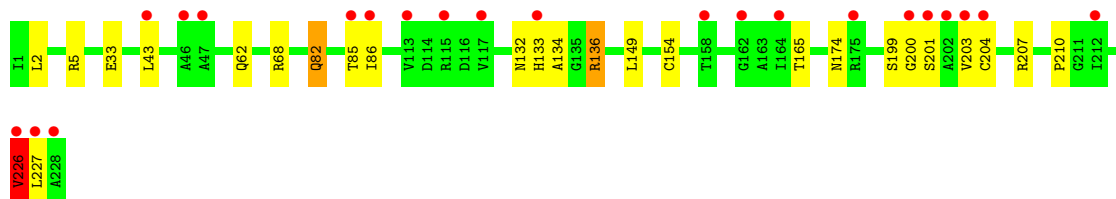
• Molecule 1: COMPLEMENT FACTOR D

Chain 74-A:



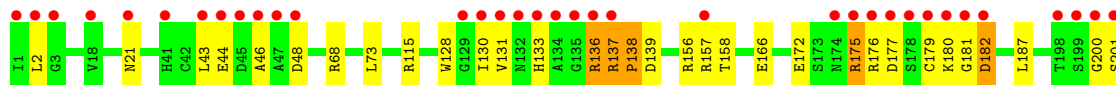
• Molecule 1: COMPLEMENT FACTOR D

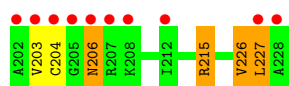
Chain 74-B:



• Molecule 1: COMPLEMENT FACTOR D

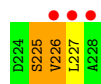
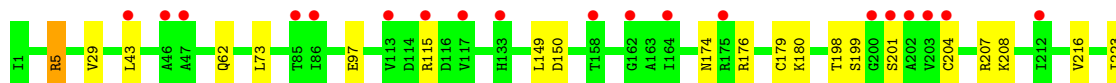
Chain 75-A:





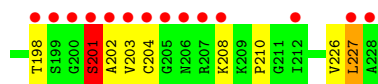
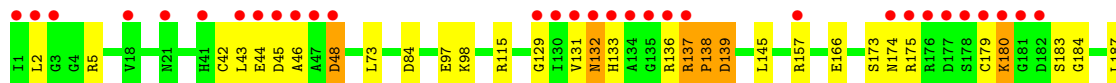
• Molecule 1: COMPLEMENT FACTOR D

Chain 75-B:



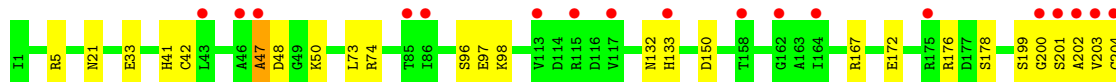
• Molecule 1: COMPLEMENT FACTOR D

Chain 76-A:



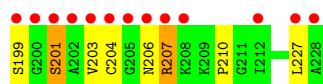
• Molecule 1: COMPLEMENT FACTOR D

Chain 76-B:



• Molecule 1: COMPLEMENT FACTOR D

Chain 77-A:



• Molecule 1: COMPLEMENT FACTOR D

Chain 77-B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Deposition
Cell constants a, b, c, α , β , γ	44.14Å 67.31Å 133.14Å 90.00° 90.00° 90.00°	Deposition
Resolution (Å)	47.33 – 1.80 47.33 – 1.80	Deposition EDS
% Data completeness (in resolution range)	98.7 (47.33-1.80) 98.7 (47.33-1.80)	Deposition EDS
R_{merge}	0.14	Deposition
R_{sym}	(Not available)	Deposition
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 1.79Å)	Xtriage
Refinement program	PHENIX (PHENIX.ENSEMBLE_REFINEMENT:DEV_1259)	Deposition
R, R_{free}	0.163 , 0.212 0.189 , 0.238	Deposition DCC
R_{free} test set	1857 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 554.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37154 reflections	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	546299	wwPDB
Average B, all atoms (Å ²)	26.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: GOL

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	1-A	0.72	0/1741	1.01	5/2370 (0.2%)
1	1-B	0.58	0/1741	0.75	2/2370 (0.1%)
1	2-A	0.77	2/1741 (0.1%)	0.97	2/2370 (0.1%)
1	2-B	0.60	1/1741 (0.1%)	0.82	1/2370 (0.0%)
1	3-A	0.80	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	3-B	0.54	0/1741	0.79	0/2370
1	4-A	0.79	3/1741 (0.2%)	1.02	7/2370 (0.3%)
1	4-B	0.56	0/1741	0.77	1/2370 (0.0%)
1	5-A	0.77	2/1741 (0.1%)	1.00	8/2370 (0.3%)
1	5-B	0.59	0/1741	0.78	1/2370 (0.0%)
1	6-A	0.74	1/1741 (0.1%)	0.99	3/2370 (0.1%)
1	6-B	0.61	0/1741	0.77	1/2370 (0.0%)
1	7-A	0.74	1/1741 (0.1%)	0.98	7/2370 (0.3%)
1	7-B	0.58	1/1741 (0.1%)	0.82	2/2370 (0.1%)
1	8-A	0.72	0/1741	1.00	6/2370 (0.3%)
1	8-B	0.58	0/1741	0.79	2/2370 (0.1%)
1	9-A	0.76	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	9-B	0.60	1/1741 (0.1%)	0.81	2/2370 (0.1%)
1	10-A	0.78	5/1741 (0.3%)	1.05	7/2370 (0.3%)
1	10-B	0.59	1/1741 (0.1%)	0.79	0/2370
1	11-A	0.74	2/1741 (0.1%)	1.03	8/2370 (0.3%)
1	11-B	0.62	0/1741	0.80	3/2370 (0.1%)
1	12-A	0.74	1/1741 (0.1%)	1.00	11/2370 (0.5%)
1	12-B	0.59	0/1741	0.80	0/2370
1	13-A	0.75	0/1741	1.00	9/2370 (0.4%)
1	13-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	14-A	0.73	1/1741 (0.1%)	0.97	6/2370 (0.3%)
1	14-B	0.59	0/1741	0.84	1/2370 (0.0%)
1	15-A	0.70	0/1741	0.96	2/2370 (0.1%)
1	15-B	0.61	0/1741	0.82	2/2370 (0.1%)
1	16-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	16-B	0.62	0/1741	0.81	0/2370

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	17-A	0.77	1/1741 (0.1%)	1.01	4/2370 (0.2%)
1	17-B	0.62	0/1741	0.83	1/2370 (0.0%)
1	18-A	0.73	2/1741 (0.1%)	0.92	3/2370 (0.1%)
1	18-B	0.60	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	19-A	0.67	0/1741	0.89	2/2370 (0.1%)
1	19-B	0.62	1/1741 (0.1%)	0.82	0/2370
1	20-A	0.79	2/1741 (0.1%)	0.97	3/2370 (0.1%)
1	20-B	0.69	3/1741 (0.2%)	0.82	1/2370 (0.0%)
1	21-A	0.71	0/1741	0.87	2/2370 (0.1%)
1	21-B	0.57	0/1741	0.76	0/2370
1	22-A	0.75	0/1741	1.02	11/2370 (0.5%)
1	22-B	0.65	1/1741 (0.1%)	0.89	5/2370 (0.2%)
1	23-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	23-B	0.66	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	24-A	0.83	4/1741 (0.2%)	1.10	9/2370 (0.4%)
1	24-B	0.68	2/1741 (0.1%)	0.83	1/2370 (0.0%)
1	25-A	0.78	0/1741	0.98	4/2370 (0.2%)
1	25-B	0.62	0/1741	0.80	0/2370
1	26-A	0.75	1/1741 (0.1%)	0.98	5/2370 (0.2%)
1	26-B	0.63	0/1741	0.83	1/2370 (0.0%)
1	27-A	0.74	0/1741	0.99	4/2370 (0.2%)
1	27-B	0.58	0/1741	0.78	0/2370
1	28-A	0.83	4/1741 (0.2%)	1.10	12/2370 (0.5%)
1	28-B	0.57	1/1741 (0.1%)	0.77	1/2370 (0.0%)
1	29-A	0.75	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	29-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	30-A	0.73	0/1741	1.00	5/2370 (0.2%)
1	30-B	0.63	0/1741	0.82	1/2370 (0.0%)
1	31-A	0.73	1/1741 (0.1%)	0.96	4/2370 (0.2%)
1	31-B	0.55	0/1741	0.76	0/2370
1	32-A	0.73	1/1741 (0.1%)	0.92	3/2370 (0.1%)
1	32-B	0.56	0/1741	0.82	5/2370 (0.2%)
1	33-A	0.76	1/1741 (0.1%)	1.00	8/2370 (0.3%)
1	33-B	0.58	0/1741	0.75	0/2370
1	34-A	0.80	5/1741 (0.3%)	0.98	6/2370 (0.3%)
1	34-B	0.59	0/1741	0.78	0/2370
1	35-A	0.70	0/1741	0.99	6/2370 (0.3%)
1	35-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	36-A	0.75	1/1741 (0.1%)	0.99	8/2370 (0.3%)
1	36-B	0.60	0/1741	0.82	2/2370 (0.1%)
1	37-A	0.71	0/1741	0.98	8/2370 (0.3%)
1	37-B	0.61	1/1741 (0.1%)	0.76	1/2370 (0.0%)
1	38-A	0.75	1/1741 (0.1%)	0.97	8/2370 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	38-B	0.62	1/1741 (0.1%)	0.84	3/2370 (0.1%)
1	39-A	0.73	0/1741	0.98	7/2370 (0.3%)
1	39-B	0.57	0/1741	0.77	2/2370 (0.1%)
1	40-A	0.71	1/1741 (0.1%)	0.91	2/2370 (0.1%)
1	40-B	0.58	0/1741	0.80	4/2370 (0.2%)
1	41-A	0.76	1/1741 (0.1%)	1.15	7/2370 (0.3%)
1	41-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	42-A	0.81	2/1741 (0.1%)	1.09	11/2370 (0.5%)
1	42-B	0.59	0/1741	0.82	1/2370 (0.0%)
1	43-A	0.78	1/1741 (0.1%)	0.98	4/2370 (0.2%)
1	43-B	0.58	0/1741	0.78	2/2370 (0.1%)
1	44-A	0.77	1/1741 (0.1%)	1.10	14/2370 (0.6%)
1	44-B	0.55	0/1741	0.78	1/2370 (0.0%)
1	45-A	0.73	0/1741	0.94	2/2370 (0.1%)
1	45-B	0.76	3/1741 (0.2%)	0.81	2/2370 (0.1%)
1	46-A	0.73	0/1741	1.01	9/2370 (0.4%)
1	46-B	0.57	0/1741	0.78	1/2370 (0.0%)
1	47-A	0.78	0/1741	0.99	5/2370 (0.2%)
1	47-B	0.60	0/1741	0.79	1/2370 (0.0%)
1	48-A	0.70	0/1741	0.97	5/2370 (0.2%)
1	48-B	0.60	1/1741 (0.1%)	0.80	0/2370
1	49-A	0.74	0/1741	1.04	9/2370 (0.4%)
1	49-B	0.61	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	50-A	0.75	1/1741 (0.1%)	0.94	6/2370 (0.3%)
1	50-B	0.59	0/1741	0.77	3/2370 (0.1%)
1	51-A	0.76	0/1741	0.99	4/2370 (0.2%)
1	51-B	0.61	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	52-A	0.75	2/1741 (0.1%)	0.97	5/2370 (0.2%)
1	52-B	0.63	1/1741 (0.1%)	0.82	4/2370 (0.2%)
1	53-A	0.79	0/1741	0.96	4/2370 (0.2%)
1	53-B	0.58	1/1741 (0.1%)	0.77	2/2370 (0.1%)
1	54-A	0.74	1/1741 (0.1%)	0.99	6/2370 (0.3%)
1	54-B	0.63	0/1741	0.81	2/2370 (0.1%)
1	55-A	0.72	1/1741 (0.1%)	1.01	6/2370 (0.3%)
1	55-B	0.58	0/1741	0.80	0/2370
1	56-A	0.74	0/1741	0.91	1/2370 (0.0%)
1	56-B	0.68	1/1741 (0.1%)	0.78	0/2370
1	57-A	0.72	0/1741	1.01	7/2370 (0.3%)
1	57-B	0.62	1/1741 (0.1%)	0.81	1/2370 (0.0%)
1	58-A	0.71	0/1741	0.98	5/2370 (0.2%)
1	58-B	0.60	1/1741 (0.1%)	0.84	2/2370 (0.1%)
1	59-A	0.72	1/1741 (0.1%)	0.90	2/2370 (0.1%)
1	59-B	0.64	3/1741 (0.2%)	0.81	2/2370 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	60-A	0.69	0/1741	0.89	3/2370 (0.1%)
1	60-B	0.63	3/1741 (0.2%)	0.81	0/2370
1	61-A	0.71	1/1741 (0.1%)	0.93	3/2370 (0.1%)
1	61-B	0.58	1/1741 (0.1%)	0.77	0/2370
1	62-A	0.71	0/1741	0.98	6/2370 (0.3%)
1	62-B	0.62	1/1741 (0.1%)	0.80	2/2370 (0.1%)
1	63-A	0.79	3/1741 (0.2%)	1.03	8/2370 (0.3%)
1	63-B	0.60	0/1741	0.84	2/2370 (0.1%)
1	64-A	0.73	0/1741	0.97	8/2370 (0.3%)
1	64-B	0.61	0/1741	0.79	2/2370 (0.1%)
1	65-A	0.72	1/1741 (0.1%)	0.94	4/2370 (0.2%)
1	65-B	0.66	1/1741 (0.1%)	0.82	3/2370 (0.1%)
1	66-A	0.73	1/1741 (0.1%)	0.89	3/2370 (0.1%)
1	66-B	0.60	1/1741 (0.1%)	0.78	1/2370 (0.0%)
1	67-A	0.76	1/1741 (0.1%)	0.95	5/2370 (0.2%)
1	67-B	0.59	1/1741 (0.1%)	0.79	2/2370 (0.1%)
1	68-A	0.79	2/1741 (0.1%)	1.01	6/2370 (0.3%)
1	68-B	0.58	1/1741 (0.1%)	0.79	1/2370 (0.0%)
1	69-A	0.79	3/1741 (0.2%)	0.95	6/2370 (0.3%)
1	69-B	0.57	0/1741	0.78	0/2370
1	70-A	0.80	4/1741 (0.2%)	0.98	4/2370 (0.2%)
1	70-B	0.64	0/1741	0.82	1/2370 (0.0%)
1	71-A	0.78	3/1741 (0.2%)	1.05	8/2370 (0.3%)
1	71-B	0.59	1/1741 (0.1%)	0.77	0/2370
1	72-A	0.75	0/1741	1.00	5/2370 (0.2%)
1	72-B	0.65	1/1741 (0.1%)	0.83	1/2370 (0.0%)
1	73-A	0.80	1/1741 (0.1%)	1.00	7/2370 (0.3%)
1	73-B	0.60	0/1741	0.78	1/2370 (0.0%)
1	74-A	0.79	2/1741 (0.1%)	1.06	8/2370 (0.3%)
1	74-B	0.66	3/1741 (0.2%)	0.78	1/2370 (0.0%)
1	75-A	0.70	0/1741	0.92	3/2370 (0.1%)
1	75-B	0.59	0/1741	0.77	0/2370
1	76-A	0.77	1/1741 (0.1%)	0.92	2/2370 (0.1%)
1	76-B	0.62	2/1741 (0.1%)	0.77	1/2370 (0.0%)
1	77-A	0.75	1/1741 (0.1%)	0.93	4/2370 (0.2%)
1	77-B	0.61	3/1741 (0.2%)	0.72	0/2370
All	All	0.68	133/268114 (0.0%)	0.90	535/364980 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-A	0	6
1	1-B	0	2
1	2-A	0	5
1	2-B	0	2
1	3-A	0	4
1	3-B	0	1
1	4-A	0	5
1	4-B	0	3
1	5-A	0	4
1	6-A	0	6
1	6-B	0	2
1	7-A	0	6
1	7-B	0	2
1	8-A	0	9
1	8-B	0	1
1	9-A	0	5
1	9-B	0	2
1	10-A	0	9
1	10-B	0	2
1	11-A	0	6
1	11-B	0	4
1	12-A	0	2
1	12-B	0	1
1	13-A	0	4
1	13-B	0	1
1	14-A	0	4
1	14-B	0	1
1	15-A	0	3
1	15-B	0	2
1	16-A	0	5
1	16-B	0	1
1	17-A	0	5
1	17-B	0	5
1	18-A	0	5
1	18-B	0	1
1	19-A	0	6
1	19-B	0	1
1	20-A	0	5
1	20-B	0	3
1	21-A	0	2
1	21-B	0	2
1	22-A	0	8
1	22-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	23-A	0	3
1	24-A	0	6
1	25-A	0	2
1	26-A	0	4
1	26-B	0	2
1	27-A	0	4
1	27-B	0	2
1	28-A	0	4
1	28-B	0	1
1	29-A	0	4
1	29-B	0	1
1	30-A	0	3
1	30-B	0	1
1	31-A	0	5
1	31-B	0	1
1	32-A	0	10
1	32-B	0	1
1	33-A	0	8
1	34-A	0	4
1	35-A	0	4
1	35-B	0	2
1	36-A	0	3
1	36-B	0	1
1	37-A	0	7
1	37-B	0	1
1	38-A	0	5
1	38-B	0	1
1	39-A	0	5
1	40-A	0	5
1	40-B	0	1
1	41-A	0	6
1	42-A	0	6
1	43-A	0	5
1	43-B	0	3
1	44-A	0	7
1	44-B	0	4
1	45-A	0	5
1	45-B	0	1
1	46-A	0	8
1	46-B	0	1
1	47-A	0	5
1	47-B	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	48-A	0	9
1	48-B	0	2
1	49-A	0	5
1	49-B	0	1
1	50-A	0	6
1	51-A	0	7
1	51-B	0	1
1	52-A	0	7
1	53-A	0	3
1	53-B	0	1
1	54-A	0	3
1	54-B	0	4
1	55-A	0	7
1	56-A	0	1
1	57-A	0	7
1	58-A	0	5
1	58-B	0	7
1	59-A	0	4
1	60-A	0	2
1	61-B	0	1
1	62-A	0	2
1	63-A	0	3
1	63-B	0	2
1	64-A	0	6
1	64-B	0	1
1	65-A	0	4
1	65-B	0	1
1	66-A	0	9
1	66-B	0	1
1	67-A	0	9
1	67-B	0	1
1	68-A	0	3
1	69-A	0	7
1	69-B	0	2
1	70-A	0	6
1	70-B	0	3
1	71-A	0	3
1	71-B	0	2
1	72-A	0	7
1	73-A	0	4
1	73-B	0	1
1	74-A	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	74-B	0	1
1	75-A	0	5
1	75-B	0	1
1	76-A	0	2
1	77-A	0	2
1	77-B	0	2
All	All	0	485

The worst 5 of 133 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	56-B	204	CYS	CB-SG	13.21	2.04	1.82
1	45-B	97	GLU	CG-CD	-12.87	1.32	1.51
1	20-A	97	GLU	CB-CG	-12.81	1.27	1.52
1	65-B	179	CYS	CB-SG	12.24	2.03	1.82
1	23-B	179	CYS	CB-SG	10.94	2.00	1.82

The worst 5 of 535 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	41-A	115	ARG	NE-CZ-NH2	-18.51	111.04	120.30
1	41-A	215	ARG	NE-CZ-NH1	16.22	128.41	120.30
1	24-A	137	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	74-A	215	ARG	NE-CZ-NH2	-14.64	112.98	120.30
1	41-A	215	ARG	NE-CZ-NH2	-14.54	113.03	120.30

There are no chirality outliers.

5 of 485 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	1	ILE	Peptide
1	1-A	131	VAL	Peptide
1	1-A	137	ARG	Peptide
1	1-A	178	SER	Peptide
1	1-A	49	GLY	Peptide

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	1-A	1706	1700	0	0	0
1	1-B	1706	1700	0	0	0
1	2-A	1706	1700	0	0	0
1	2-B	1706	1700	0	0	1
1	3-A	1706	1700	0	0	0
1	3-B	1706	1700	0	0	1
1	4-A	1706	1700	0	0	2
1	4-B	1706	1700	0	0	1
1	5-A	1706	1700	0	0	0
1	5-B	1706	1700	0	0	1
1	6-A	1706	1700	0	0	1
1	6-B	1706	1700	0	0	0
1	7-A	1706	1700	0	0	0
1	7-B	1706	1700	0	0	0
1	8-A	1706	1700	0	0	0
1	8-B	1706	1700	0	0	0
1	9-A	1706	1700	0	0	0
1	9-B	1706	1700	0	0	0
1	10-A	1706	1700	0	0	0
1	10-B	1706	1700	0	0	0
1	11-A	1706	1700	0	0	1
1	11-B	1706	1700	0	0	0
1	12-A	1706	1700	0	0	1
1	12-B	1706	1700	0	0	0
1	13-A	1706	1700	0	0	0
1	13-B	1706	1700	0	0	0
1	14-A	1706	1700	0	0	1
1	14-B	1706	1700	0	0	0
1	15-A	1706	1700	0	0	1
1	15-B	1706	1700	0	0	1
1	16-A	1706	1700	0	0	1
1	16-B	1706	1700	0	0	1
1	17-A	1706	1700	0	0	0
1	17-B	1706	1700	0	0	2
1	18-A	1706	1700	0	0	0
1	18-B	1706	1700	0	0	2
1	19-A	1706	1700	0	0	1
1	19-B	1706	1700	0	0	0
1	20-A	1706	1700	0	0	0
1	20-B	1706	1700	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	21-A	1706	1700	0	0	0
1	21-B	1706	1700	0	0	1
1	22-A	1706	1700	0	0	1
1	22-B	1706	1700	0	0	1
1	23-A	1706	1700	0	0	0
1	23-B	1706	1700	0	0	0
1	24-A	1706	1700	0	0	0
1	24-B	1706	1700	0	0	1
1	25-A	1706	1700	0	0	0
1	25-B	1706	1700	0	0	0
1	26-A	1706	1700	0	0	1
1	26-B	1706	1700	0	0	0
1	27-A	1706	1700	0	0	0
1	27-B	1706	1700	0	0	1
1	28-A	1706	1700	0	0	1
1	28-B	1706	1700	0	0	2
1	29-A	1706	1700	0	0	2
1	29-B	1706	1700	0	0	0
1	30-A	1706	1700	0	0	1
1	30-B	1706	1700	0	0	0
1	31-A	1706	1700	0	0	0
1	31-B	1706	1700	0	0	0
1	32-A	1706	1700	0	0	0
1	32-B	1706	1700	0	0	0
1	33-A	1706	1700	0	0	1
1	33-B	1706	1700	0	0	1
1	34-A	1706	1700	0	0	1
1	34-B	1706	1700	0	0	0
1	35-A	1706	1700	0	0	0
1	35-B	1706	1700	0	0	1
1	36-A	1706	1700	0	0	0
1	36-B	1706	1700	0	0	1
1	37-A	1706	1700	0	0	1
1	37-B	1706	1700	0	0	0
1	38-A	1706	1700	0	0	0
1	38-B	1706	1700	0	0	0
1	39-A	1706	1700	0	0	2
1	39-B	1706	1700	0	0	1
1	40-A	1706	1700	0	0	1
1	40-B	1706	1700	0	0	0
1	41-A	1706	1700	0	0	1
1	41-B	1706	1700	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	42-A	1706	1700	0	0	1
1	42-B	1706	1700	0	0	1
1	43-A	1706	1700	0	0	0
1	43-B	1706	1700	0	0	0
1	44-A	1706	1700	0	0	1
1	44-B	1706	1700	0	0	0
1	45-A	1706	1700	0	0	0
1	45-B	1706	1700	0	0	0
1	46-A	1706	1700	0	0	0
1	46-B	1706	1700	0	0	0
1	47-A	1706	1700	0	0	1
1	47-B	1706	1700	0	0	1
1	48-A	1706	1700	0	0	0
1	48-B	1706	1700	0	0	0
1	49-A	1706	1700	0	0	0
1	49-B	1706	1700	0	0	0
1	50-A	1706	1700	0	0	0
1	50-B	1706	1700	0	0	1
1	51-A	1706	1700	0	0	0
1	51-B	1706	1700	0	0	1
1	52-A	1706	1700	0	0	0
1	52-B	1706	1700	0	0	0
1	53-A	1706	1700	0	0	0
1	53-B	1706	1700	0	0	0
1	54-A	1706	1700	0	0	1
1	54-B	1706	1700	0	0	0
1	55-A	1706	1700	0	0	1
1	55-B	1706	1700	0	0	2
1	56-A	1706	1700	0	0	0
1	56-B	1706	1700	0	0	1
1	57-A	1706	1700	0	0	0
1	57-B	1706	1700	0	0	0
1	58-A	1706	1700	0	0	0
1	58-B	1706	1700	0	0	0
1	59-A	1706	1700	0	0	0
1	59-B	1706	1700	0	0	0
1	60-A	1706	1700	0	0	0
1	60-B	1706	1700	0	0	0
1	61-A	1706	1700	0	0	2
1	61-B	1706	1700	0	0	1
1	62-A	1706	1700	0	0	0
1	62-B	1706	1700	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	63-A	1706	1700	0	0	0
1	63-B	1706	1700	0	0	1
1	64-A	1706	1700	0	0	1
1	64-B	1706	1700	0	0	0
1	65-A	1706	1700	0	0	0
1	65-B	1706	1700	0	0	0
1	66-A	1706	1700	0	0	0
1	66-B	1706	1700	0	0	1
1	67-A	1706	1700	0	0	0
1	67-B	1706	1700	0	0	0
1	68-A	1706	1700	0	0	1
1	68-B	1706	1700	0	0	0
1	69-A	1706	1700	0	0	1
1	69-B	1706	1700	0	0	0
1	70-A	1706	1700	0	0	0
1	70-B	1706	1700	0	0	1
1	71-A	1706	1700	0	0	1
1	71-B	1706	1700	0	0	1
1	72-A	1706	1700	0	0	0
1	72-B	1706	1700	0	0	1
1	73-A	1706	1700	0	0	1
1	73-B	1706	1700	0	0	0
1	74-A	1706	1700	0	0	0
1	74-B	1706	1700	0	0	1
1	75-A	1706	1700	0	0	1
1	75-B	1706	1700	0	0	1
1	76-A	1706	1700	0	0	2
1	76-B	1706	1700	0	0	2
1	77-A	1706	1700	0	0	2
1	77-B	1706	1700	0	0	3
2	1-A	6	8	0	0	0
2	1-B	6	8	0	0	0
2	2-A	6	8	0	0	0
2	2-B	6	8	0	0	0
2	3-A	6	8	0	0	0
2	3-B	6	8	0	0	0
2	4-A	6	8	0	0	0
2	4-B	6	8	0	0	0
2	5-A	6	8	0	0	0
2	5-B	6	8	0	0	0
2	6-A	6	8	0	0	0
2	6-B	6	8	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	7-A	6	8	0	0	0
2	7-B	6	8	0	0	0
2	8-A	6	8	0	0	0
2	8-B	6	8	0	0	0
2	9-A	6	8	0	0	0
2	9-B	6	8	0	0	0
2	10-A	6	8	0	0	0
2	10-B	6	8	0	0	0
2	11-A	6	8	0	0	0
2	11-B	6	8	0	0	0
2	12-A	6	8	0	0	0
2	12-B	6	8	0	0	0
2	13-A	6	8	0	0	0
2	13-B	6	8	0	0	0
2	14-A	6	8	0	0	0
2	14-B	6	8	0	0	0
2	15-A	6	8	0	0	0
2	15-B	6	8	0	0	0
2	16-A	6	8	0	0	0
2	16-B	6	8	0	0	0
2	17-A	6	8	0	0	0
2	17-B	6	8	0	0	0
2	18-A	6	8	0	0	0
2	18-B	6	8	0	0	0
2	19-A	6	8	0	0	0
2	19-B	6	8	0	0	0
2	20-A	6	8	0	0	0
2	20-B	6	8	0	0	0
2	21-A	6	8	0	0	0
2	21-B	6	8	0	0	0
2	22-A	6	8	0	0	0
2	22-B	6	8	0	0	0
2	23-A	6	8	0	0	0
2	23-B	6	8	0	0	0
2	24-A	6	8	0	0	0
2	24-B	6	8	0	0	0
2	25-A	6	8	0	0	0
2	25-B	6	8	0	0	0
2	26-A	6	8	0	0	0
2	26-B	6	8	0	0	0
2	27-A	6	8	0	0	0
2	27-B	6	8	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	28-A	6	8	0	0	0
2	28-B	6	8	0	0	0
2	29-A	6	8	0	0	0
2	29-B	6	8	0	0	0
2	30-A	6	8	0	0	0
2	30-B	6	8	0	0	0
2	31-A	6	8	0	0	0
2	31-B	6	8	0	0	0
2	32-A	6	8	0	0	0
2	32-B	6	8	0	0	0
2	33-A	6	8	0	0	0
2	33-B	6	8	0	0	0
2	34-A	6	8	0	0	0
2	34-B	6	8	0	0	0
2	35-A	6	8	0	0	0
2	35-B	6	8	0	0	0
2	36-A	6	8	0	0	0
2	36-B	6	8	0	0	0
2	37-A	6	8	0	0	0
2	37-B	6	8	0	0	0
2	38-A	6	8	0	0	0
2	38-B	6	8	0	0	0
2	39-A	6	8	0	0	0
2	39-B	6	8	0	0	0
2	40-A	6	8	0	0	0
2	40-B	6	8	0	0	0
2	41-A	6	8	0	0	0
2	41-B	6	8	0	0	0
2	42-A	6	8	0	0	0
2	42-B	6	8	0	0	0
2	43-A	6	8	0	0	0
2	43-B	6	8	0	0	0
2	44-A	6	8	0	0	0
2	44-B	6	8	0	0	0
2	45-A	6	8	0	0	0
2	45-B	6	8	0	0	0
2	46-A	6	8	0	0	0
2	46-B	6	8	0	0	0
2	47-A	6	8	0	0	0
2	47-B	6	8	0	0	0
2	48-A	6	8	0	0	0
2	48-B	6	8	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	49-A	6	8	0	0	0
2	49-B	6	8	0	0	0
2	50-A	6	8	0	0	0
2	50-B	6	8	0	0	0
2	51-A	6	8	0	0	0
2	51-B	6	8	0	0	0
2	52-A	6	8	0	0	0
2	52-B	6	8	0	0	0
2	53-A	6	8	0	0	0
2	53-B	6	8	0	0	0
2	54-A	6	8	0	0	0
2	54-B	6	8	0	0	0
2	55-A	6	8	0	0	0
2	55-B	6	8	0	0	0
2	56-A	6	8	0	0	0
2	56-B	6	8	0	0	0
2	57-A	6	8	0	0	0
2	57-B	6	8	0	0	0
2	58-A	6	8	0	0	0
2	58-B	6	8	0	0	0
2	59-A	6	8	0	0	0
2	59-B	6	8	0	0	0
2	60-A	6	8	0	0	0
2	60-B	6	8	0	0	0
2	61-A	6	8	0	0	0
2	61-B	6	8	0	0	0
2	62-A	6	8	0	0	0
2	62-B	6	8	0	0	0
2	63-A	6	8	0	0	0
2	63-B	6	8	0	0	0
2	64-A	6	8	0	0	0
2	64-B	6	8	0	0	0
2	65-A	6	8	0	0	0
2	65-B	6	8	0	0	0
2	66-A	6	8	0	0	0
2	66-B	6	8	0	0	0
2	67-A	6	8	0	0	0
2	67-B	6	8	0	0	0
2	68-A	6	8	0	0	0
2	68-B	6	8	0	0	0
2	69-A	6	8	0	0	0
2	69-B	6	8	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	70-A	6	8	0	0	0
2	70-B	6	8	0	0	0
2	71-A	6	8	0	0	0
2	71-B	6	8	0	0	0
2	72-A	6	8	0	0	0
2	72-B	6	8	0	0	0
2	73-A	6	8	0	0	0
2	73-B	6	8	0	0	0
2	74-A	6	8	0	0	0
2	74-B	6	8	0	0	0
2	75-A	6	8	0	0	0
2	75-B	6	8	0	0	0
2	76-A	6	8	0	0	0
2	76-B	6	8	0	0	0
2	77-A	6	8	0	0	0
2	77-B	6	8	0	0	0
3	1-A	148	0	0	0	1
3	1-B	113	0	0	0	0
3	2-A	139	0	0	0	2
3	2-B	122	0	0	0	1
3	3-A	142	0	0	0	1
3	3-B	96	0	0	0	0
3	4-A	129	0	0	0	1
3	4-B	108	0	0	0	1
3	5-A	129	0	0	0	1
3	5-B	109	0	0	0	1
3	6-A	136	0	0	0	0
3	6-B	111	0	0	0	0
3	7-A	134	0	0	0	0
3	7-B	111	0	0	0	0
3	8-A	136	0	0	0	3
3	8-B	104	0	0	0	1
3	9-A	138	0	0	0	1
3	9-B	119	0	0	0	0
3	10-A	135	0	0	0	0
3	10-B	117	0	0	0	0
3	11-A	123	0	0	0	2
3	11-B	118	0	0	0	2
3	12-A	145	0	0	0	0
3	12-B	115	0	0	0	1
3	13-A	165	0	0	0	2
3	13-B	109	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	14-A	157	0	0	0	1
3	14-B	115	0	0	0	0
3	15-A	142	0	0	0	1
3	15-B	113	0	0	0	1
3	16-A	135	0	0	0	3
3	16-B	117	0	0	0	3
3	17-A	142	0	0	0	4
3	17-B	122	0	0	0	3
3	18-A	147	0	0	0	1
3	18-B	111	0	0	0	0
3	19-A	127	0	0	0	2
3	19-B	117	0	0	0	3
3	20-A	131	0	0	0	1
3	20-B	123	0	0	0	1
3	21-A	144	0	0	0	0
3	21-B	103	0	0	0	0
3	22-A	143	0	0	0	1
3	22-B	122	0	0	0	0
3	23-A	142	0	0	0	0
3	23-B	113	0	0	0	0
3	24-A	127	0	0	0	1
3	24-B	116	0	0	0	0
3	25-A	137	0	0	0	1
3	25-B	120	0	0	0	1
3	26-A	145	0	0	0	1
3	26-B	114	0	0	0	1
3	27-A	139	0	0	0	1
3	27-B	114	0	0	0	0
3	28-A	137	0	0	0	1
3	28-B	123	0	0	0	0
3	29-A	135	0	0	0	3
3	29-B	132	0	0	0	3
3	30-A	149	0	0	0	1
3	30-B	115	0	0	0	2
3	31-A	146	0	0	0	0
3	31-B	117	0	0	0	0
3	32-A	135	0	0	0	1
3	32-B	127	0	0	0	1
3	33-A	133	0	0	0	1
3	33-B	119	0	0	0	0
3	34-A	139	0	0	0	0
3	34-B	109	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	35-A	125	0	0	0	4
3	35-B	102	0	0	0	2
3	36-A	130	0	0	0	1
3	36-B	120	0	0	0	1
3	37-A	138	0	0	0	2
3	37-B	110	0	0	0	1
3	38-A	134	0	0	0	0
3	38-B	118	0	0	0	0
3	39-A	130	0	0	0	1
3	39-B	112	0	0	0	2
3	40-A	128	0	0	0	0
3	40-B	118	0	0	0	0
3	41-A	139	0	0	0	3
3	41-B	106	0	0	0	1
3	42-A	128	0	0	0	0
3	42-B	124	0	0	0	0
3	43-A	155	0	0	0	0
3	43-B	125	0	0	0	0
3	44-A	143	0	0	0	0
3	44-B	118	0	0	0	0
3	45-A	140	0	0	0	3
3	45-B	108	0	0	0	3
3	46-A	131	0	0	0	1
3	46-B	105	0	0	0	1
3	47-A	127	0	0	0	0
3	47-B	118	0	0	0	0
3	48-A	141	0	0	0	1
3	48-B	129	0	0	0	1
3	49-A	121	0	0	0	0
3	49-B	109	0	0	0	0
3	50-A	139	0	0	0	2
3	50-B	111	0	0	0	0
3	51-A	137	0	0	0	2
3	51-B	131	0	0	0	0
3	52-A	145	0	0	0	1
3	52-B	119	0	0	0	1
3	53-A	141	0	0	0	2
3	53-B	113	0	0	0	1
3	54-A	137	0	0	0	5
3	54-B	109	0	0	0	3
3	55-A	136	0	0	0	0
3	55-B	120	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	56-A	153	0	0	0	1
3	56-B	127	0	0	0	0
3	57-A	124	0	0	0	0
3	57-B	122	0	0	0	0
3	58-A	133	0	0	0	1
3	58-B	122	0	0	0	1
3	59-A	143	0	0	0	0
3	59-B	117	0	0	0	0
3	60-A	132	0	0	0	0
3	60-B	116	0	0	0	0
3	61-A	138	0	0	0	1
3	61-B	119	0	0	0	1
3	62-A	137	0	0	0	2
3	62-B	121	0	0	0	2
3	63-A	151	0	0	0	2
3	63-B	123	0	0	0	1
3	64-A	142	0	0	0	0
3	64-B	121	0	0	0	1
3	65-A	149	0	0	0	1
3	65-B	128	0	0	0	1
3	66-A	135	0	0	0	1
3	66-B	112	0	0	0	2
3	67-A	143	0	0	0	0
3	67-B	125	0	0	0	0
3	68-A	137	0	0	0	2
3	68-B	126	0	0	0	3
3	69-A	131	0	0	0	0
3	69-B	112	0	0	0	0
3	70-A	136	0	0	0	2
3	70-B	123	0	0	0	2
3	71-A	138	0	0	0	1
3	71-B	122	0	0	0	0
3	72-A	135	0	0	0	0
3	72-B	121	0	0	0	0
3	73-A	134	0	0	0	3
3	73-B	132	0	0	0	5
3	74-A	153	0	0	0	1
3	74-B	113	0	0	0	0
3	75-A	147	0	0	0	1
3	75-B	111	0	0	0	1
3	76-A	145	0	0	0	0
3	76-B	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	77-A	131	0	0	0	3
3	77-B	119	0	0	0	0
All	All	283267	263032	0	0	140

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

The worst 5 of 140 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)
3:A:1186:HOH:O	3:B:1219:HOH:O[3_454]	0.19	2.01
3:A:1190:HOH:O	3:B:1212:HOH:O[3_554]	0.62	1.58
3:A:1166:HOH:O	3:B:1218[A]:HOH:O[3_454]	0.87	1.33
3:A:1238:HOH:O	3:B:1167:HOH:O[3_544]	0.97	1.23
3:A:1175:HOH:O	3:A:1225:HOH:O[1_455]	1.54	0.66

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	1-A	226/228 (99%)	191 (84%)	19 (8%)	16 (7%)	2	0
1	1-B	226/228 (99%)	203 (90%)	15 (7%)	8 (4%)	6	0
1	2-A	226/228 (99%)	184 (81%)	15 (7%)	27 (12%)	1	0
1	2-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	3	0
1	3-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	2	0
1	3-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	5	0
1	4-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	1	0
1	4-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0
1	5-A	226/228 (99%)	187 (83%)	24 (11%)	15 (7%)	2	0
1	5-B	226/228 (99%)	198 (88%)	24 (11%)	4 (2%)	13	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	6-A	226/228 (99%)	185 (82%)	26 (12%)	15 (7%)	2	0
1	6-B	226/228 (99%)	201 (89%)	18 (8%)	7 (3%)	7	0
1	7-A	226/228 (99%)	180 (80%)	21 (9%)	25 (11%)	1	0
1	7-B	226/228 (99%)	204 (90%)	18 (8%)	4 (2%)	13	2
1	8-A	226/228 (99%)	185 (82%)	18 (8%)	23 (10%)	1	0
1	8-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	6	0
1	9-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	9-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	4	0
1	10-A	226/228 (99%)	176 (78%)	28 (12%)	22 (10%)	1	0
1	10-B	226/228 (99%)	203 (90%)	19 (8%)	4 (2%)	13	2
1	11-A	226/228 (99%)	185 (82%)	25 (11%)	16 (7%)	2	0
1	11-B	226/228 (99%)	205 (91%)	15 (7%)	6 (3%)	8	1
1	12-A	226/228 (99%)	182 (80%)	21 (9%)	23 (10%)	1	0
1	12-B	226/228 (99%)	197 (87%)	15 (7%)	14 (6%)	2	0
1	13-A	226/228 (99%)	191 (84%)	17 (8%)	18 (8%)	1	0
1	13-B	226/228 (99%)	199 (88%)	20 (9%)	7 (3%)	7	0
1	14-A	226/228 (99%)	193 (85%)	11 (5%)	22 (10%)	1	0
1	14-B	226/228 (99%)	206 (91%)	14 (6%)	6 (3%)	8	1
1	15-A	226/228 (99%)	181 (80%)	21 (9%)	24 (11%)	1	0
1	15-B	226/228 (99%)	200 (88%)	20 (9%)	6 (3%)	8	1
1	16-A	226/228 (99%)	186 (82%)	20 (9%)	20 (9%)	1	0
1	16-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	4	0
1	17-A	226/228 (99%)	189 (84%)	14 (6%)	23 (10%)	1	0
1	17-B	226/228 (99%)	187 (83%)	26 (12%)	13 (6%)	3	0
1	18-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	2	0
1	18-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	5	0
1	19-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	2	0
1	19-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	3	0
1	20-A	226/228 (99%)	190 (84%)	25 (11%)	11 (5%)	3	0
1	20-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	4	0
1	21-A	226/228 (99%)	189 (84%)	25 (11%)	12 (5%)	3	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	21-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	4	0
1	22-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	2	0
1	22-B	226/228 (99%)	198 (88%)	16 (7%)	12 (5%)	3	0
1	23-A	226/228 (99%)	189 (84%)	21 (9%)	16 (7%)	2	0
1	23-B	226/228 (99%)	200 (88%)	16 (7%)	10 (4%)	4	0
1	24-A	226/228 (99%)	183 (81%)	26 (12%)	17 (8%)	2	0
1	24-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	8	1
1	25-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	3	0
1	25-B	226/228 (99%)	202 (89%)	18 (8%)	6 (3%)	8	1
1	26-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	2	0
1	26-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	4	0
1	27-A	226/228 (99%)	184 (81%)	20 (9%)	22 (10%)	1	0
1	27-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0
1	28-A	226/228 (99%)	183 (81%)	24 (11%)	19 (8%)	1	0
1	28-B	226/228 (99%)	198 (88%)	17 (8%)	11 (5%)	3	0
1	29-A	226/228 (99%)	187 (83%)	27 (12%)	12 (5%)	3	0
1	29-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	7	0
1	30-A	226/228 (99%)	195 (86%)	21 (9%)	10 (4%)	4	0
1	30-B	226/228 (99%)	201 (89%)	17 (8%)	8 (4%)	6	0
1	31-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	31-B	226/228 (99%)	207 (92%)	9 (4%)	10 (4%)	4	0
1	32-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	2	0
1	32-B	226/228 (99%)	202 (89%)	15 (7%)	9 (4%)	5	0
1	33-A	226/228 (99%)	193 (85%)	20 (9%)	13 (6%)	3	0
1	33-B	226/228 (99%)	203 (90%)	13 (6%)	10 (4%)	4	0
1	34-A	226/228 (99%)	189 (84%)	23 (10%)	14 (6%)	2	0
1	34-B	226/228 (99%)	198 (88%)	18 (8%)	10 (4%)	4	0
1	35-A	226/228 (99%)	188 (83%)	25 (11%)	13 (6%)	3	0
1	35-B	226/228 (99%)	201 (89%)	15 (7%)	10 (4%)	4	0
1	36-A	226/228 (99%)	186 (82%)	22 (10%)	18 (8%)	1	0
1	36-B	226/228 (99%)	206 (91%)	11 (5%)	9 (4%)	5	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	37-A	226/228 (99%)	181 (80%)	23 (10%)	22 (10%)	1	0
1	37-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	6	0
1	38-A	226/228 (99%)	183 (81%)	22 (10%)	21 (9%)	1	0
1	38-B	226/228 (99%)	200 (88%)	17 (8%)	9 (4%)	5	0
1	39-A	226/228 (99%)	190 (84%)	18 (8%)	18 (8%)	1	0
1	39-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	6	0
1	40-A	226/228 (99%)	186 (82%)	28 (12%)	12 (5%)	3	0
1	40-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0
1	41-A	226/228 (99%)	185 (82%)	16 (7%)	25 (11%)	1	0
1	41-B	226/228 (99%)	201 (89%)	19 (8%)	6 (3%)	8	1
1	42-A	226/228 (99%)	186 (82%)	19 (8%)	21 (9%)	1	0
1	42-B	226/228 (99%)	199 (88%)	23 (10%)	4 (2%)	13	2
1	43-A	226/228 (99%)	189 (84%)	20 (9%)	17 (8%)	2	0
1	43-B	226/228 (99%)	197 (87%)	20 (9%)	9 (4%)	5	0
1	44-A	226/228 (99%)	184 (81%)	24 (11%)	18 (8%)	1	0
1	44-B	226/228 (99%)	204 (90%)	13 (6%)	9 (4%)	5	0
1	45-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	45-B	226/228 (99%)	203 (90%)	14 (6%)	9 (4%)	5	0
1	46-A	226/228 (99%)	182 (80%)	27 (12%)	17 (8%)	2	0
1	46-B	226/228 (99%)	198 (88%)	15 (7%)	13 (6%)	3	0
1	47-A	226/228 (99%)	182 (80%)	22 (10%)	22 (10%)	1	0
1	47-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0
1	48-A	226/228 (99%)	184 (81%)	26 (12%)	16 (7%)	2	0
1	48-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	7	0
1	49-A	226/228 (99%)	181 (80%)	25 (11%)	20 (9%)	1	0
1	49-B	226/228 (99%)	201 (89%)	16 (7%)	9 (4%)	5	0
1	50-A	226/228 (99%)	185 (82%)	22 (10%)	19 (8%)	1	0
1	50-B	226/228 (99%)	196 (87%)	22 (10%)	8 (4%)	6	0
1	51-A	226/228 (99%)	190 (84%)	17 (8%)	19 (8%)	1	0
1	51-B	226/228 (99%)	195 (86%)	20 (9%)	11 (5%)	3	0
1	52-A	226/228 (99%)	182 (80%)	26 (12%)	18 (8%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	52-B	226/228 (99%)	206 (91%)	13 (6%)	7 (3%)	7	0
1	53-A	226/228 (99%)	185 (82%)	28 (12%)	13 (6%)	3	0
1	53-B	226/228 (99%)	204 (90%)	14 (6%)	8 (4%)	6	0
1	54-A	226/228 (99%)	188 (83%)	21 (9%)	17 (8%)	2	0
1	54-B	226/228 (99%)	200 (88%)	19 (8%)	7 (3%)	7	0
1	55-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	55-B	226/228 (99%)	197 (87%)	18 (8%)	11 (5%)	3	0
1	56-A	226/228 (99%)	191 (84%)	23 (10%)	12 (5%)	3	0
1	56-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	6	0
1	57-A	226/228 (99%)	184 (81%)	19 (8%)	23 (10%)	1	0
1	57-B	226/228 (99%)	195 (86%)	23 (10%)	8 (4%)	6	0
1	58-A	226/228 (99%)	189 (84%)	16 (7%)	21 (9%)	1	0
1	58-B	226/228 (99%)	201 (89%)	11 (5%)	14 (6%)	2	0
1	59-A	226/228 (99%)	193 (85%)	14 (6%)	19 (8%)	1	0
1	59-B	226/228 (99%)	199 (88%)	19 (8%)	8 (4%)	6	0
1	60-A	226/228 (99%)	186 (82%)	23 (10%)	17 (8%)	2	0
1	60-B	226/228 (99%)	197 (87%)	16 (7%)	13 (6%)	3	0
1	61-A	226/228 (99%)	177 (78%)	28 (12%)	21 (9%)	1	0
1	61-B	226/228 (99%)	203 (90%)	10 (4%)	13 (6%)	3	0
1	62-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	2	0
1	62-B	226/228 (99%)	202 (89%)	17 (8%)	7 (3%)	7	0
1	63-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	2	0
1	63-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	6	0
1	64-A	226/228 (99%)	183 (81%)	20 (9%)	23 (10%)	1	0
1	64-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0
1	65-A	226/228 (99%)	187 (83%)	22 (10%)	17 (8%)	2	0
1	65-B	226/228 (99%)	198 (88%)	21 (9%)	7 (3%)	7	0
1	66-A	226/228 (99%)	192 (85%)	21 (9%)	13 (6%)	3	0
1	66-B	226/228 (99%)	202 (89%)	16 (7%)	8 (4%)	6	0
1	67-A	226/228 (99%)	185 (82%)	24 (11%)	17 (8%)	2	0
1	67-B	226/228 (99%)	200 (88%)	18 (8%)	8 (4%)	6	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	68-A	226/228 (99%)	179 (79%)	23 (10%)	24 (11%)	1	0
1	68-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	4	0
1	69-A	226/228 (99%)	184 (81%)	28 (12%)	14 (6%)	2	0
1	69-B	226/228 (99%)	195 (86%)	18 (8%)	13 (6%)	3	0
1	70-A	226/228 (99%)	186 (82%)	24 (11%)	16 (7%)	2	0
1	70-B	226/228 (99%)	202 (89%)	14 (6%)	10 (4%)	4	0
1	71-A	226/228 (99%)	184 (81%)	27 (12%)	15 (7%)	2	0
1	71-B	226/228 (99%)	197 (87%)	22 (10%)	7 (3%)	7	0
1	72-A	226/228 (99%)	183 (81%)	30 (13%)	13 (6%)	3	0
1	72-B	226/228 (99%)	207 (92%)	14 (6%)	5 (2%)	10	1
1	73-A	226/228 (99%)	185 (82%)	21 (9%)	20 (9%)	1	0
1	73-B	226/228 (99%)	203 (90%)	18 (8%)	5 (2%)	10	1
1	74-A	226/228 (99%)	187 (83%)	20 (9%)	19 (8%)	1	0
1	74-B	226/228 (99%)	205 (91%)	13 (6%)	8 (4%)	6	0
1	75-A	226/228 (99%)	185 (82%)	23 (10%)	18 (8%)	1	0
1	75-B	226/228 (99%)	200 (88%)	23 (10%)	3 (1%)	18	4
1	76-A	226/228 (99%)	190 (84%)	19 (8%)	17 (8%)	2	0
1	76-B	226/228 (99%)	207 (92%)	13 (6%)	6 (3%)	8	1
1	77-A	226/228 (99%)	183 (81%)	25 (11%)	18 (8%)	1	0
1	77-B	226/228 (99%)	197 (87%)	19 (8%)	10 (4%)	4	0
All	All	34804/35112 (99%)	29722 (85%)	3047 (9%)	2035 (6%)	3	0

5 of 2035 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	45	ASP
1	1-A	131	VAL
1	1-A	134	ALA
1	1-A	180	LYS
1	1-A	206	ASN

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	1-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	1-B	181/181 (100%)	166 (92%)	15 (8%)	16	4
1	2-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	2-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	3-A	181/181 (100%)	153 (84%)	28 (16%)	4	0
1	3-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	4-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	4-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	5-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	5-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	6-A	181/181 (100%)	152 (84%)	29 (16%)	3	0
1	6-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	7-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	7-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	8-A	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	8-B	181/181 (100%)	166 (92%)	15 (8%)	16	4
1	9-A	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	9-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	10-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	10-B	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	11-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	11-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	12-A	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	12-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	13-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	13-B	181/181 (100%)	167 (92%)	14 (8%)	18	5
1	14-A	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	14-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	15-A	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	15-B	181/181 (100%)	160 (88%)	21 (12%)	8	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	16-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	16-B	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	17-A	181/181 (100%)	150 (83%)	31 (17%)	3	0
1	17-B	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	18-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	18-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	19-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	19-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	20-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	20-B	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	21-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	21-B	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	22-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	22-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	23-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	23-B	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	24-A	181/181 (100%)	149 (82%)	32 (18%)	3	0
1	24-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	25-A	181/181 (100%)	150 (83%)	31 (17%)	3	0
1	25-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	26-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	26-B	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	27-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	27-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	28-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	28-B	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	29-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	29-B	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	30-A	181/181 (100%)	152 (84%)	29 (16%)	3	0
1	30-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	31-A	181/181 (100%)	156 (86%)	25 (14%)	5	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	31-B	181/181 (100%)	167 (92%)	14 (8%)	18	5
1	32-A	181/181 (100%)	151 (83%)	30 (17%)	3	0
1	32-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	33-A	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	33-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	34-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	34-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	35-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	35-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	36-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	36-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	37-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	37-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	38-A	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	38-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	39-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	39-B	181/181 (100%)	166 (92%)	15 (8%)	16	4
1	40-A	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	40-B	181/181 (100%)	167 (92%)	14 (8%)	18	5
1	41-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	41-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	42-A	181/181 (100%)	153 (84%)	28 (16%)	4	0
1	42-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	43-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	43-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	44-A	181/181 (100%)	147 (81%)	34 (19%)	2	0
1	44-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	45-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	45-B	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	46-A	181/181 (100%)	146 (81%)	35 (19%)	2	0
1	46-B	181/181 (100%)	166 (92%)	15 (8%)	16	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	47-A	181/181 (100%)	153 (84%)	28 (16%)	4	0
1	47-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	48-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	48-B	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	49-A	181/181 (100%)	153 (84%)	28 (16%)	4	0
1	49-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	50-A	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	50-B	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	51-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	51-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	52-A	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	52-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	53-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	53-B	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	54-A	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	54-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	55-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	55-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	56-A	181/181 (100%)	151 (83%)	30 (17%)	3	0
1	56-B	181/181 (100%)	166 (92%)	15 (8%)	16	4
1	57-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	57-B	181/181 (100%)	166 (92%)	15 (8%)	16	4
1	58-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	58-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	59-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	59-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	60-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	60-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	61-A	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	61-B	181/181 (100%)	153 (84%)	28 (16%)	4	0
1	62-A	181/181 (100%)	159 (88%)	22 (12%)	7	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	62-B	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	63-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	63-B	181/181 (100%)	168 (93%)	13 (7%)	21	6
1	64-A	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	64-B	181/181 (100%)	157 (87%)	24 (13%)	6	1
1	65-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	65-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	66-A	181/181 (100%)	150 (83%)	31 (17%)	3	0
1	66-B	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	67-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	67-B	181/181 (100%)	169 (93%)	12 (7%)	24	8
1	68-A	181/181 (100%)	152 (84%)	29 (16%)	3	0
1	68-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	69-A	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	69-B	181/181 (100%)	163 (90%)	18 (10%)	11	3
1	70-A	181/181 (100%)	158 (87%)	23 (13%)	6	1
1	70-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	71-A	181/181 (100%)	154 (85%)	27 (15%)	4	1
1	71-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	72-A	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	72-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	73-A	181/181 (100%)	155 (86%)	26 (14%)	5	1
1	73-B	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	74-A	181/181 (100%)	164 (91%)	17 (9%)	13	3
1	74-B	181/181 (100%)	165 (91%)	16 (9%)	14	4
1	75-A	181/181 (100%)	160 (88%)	21 (12%)	8	1
1	75-B	181/181 (100%)	159 (88%)	22 (12%)	7	1
1	76-A	181/181 (100%)	156 (86%)	25 (14%)	5	1
1	76-B	181/181 (100%)	161 (89%)	20 (11%)	9	2
1	77-A	181/181 (100%)	162 (90%)	19 (10%)	10	2
1	77-B	181/181 (100%)	166 (92%)	15 (8%)	16	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	27874/27874 (100%)	24533 (88%)	3341 (12%)	7 1

5 of 3341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	35-A	48	ASP
1	43-B	175	ARG
1	71-B	48	ASP
1	36-A	85	THR
1	39-B	44	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

154 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	1-A	1000	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	1-B	1000	-	5,5,5	0.21	0	5,5,5	0.29	0
2	GOL	10-A	1000	-	5,5,5	0.29	0	5,5,5	1.25	0
2	GOL	10-B	1000	-	5,5,5	0.20	0	5,5,5	0.40	0
2	GOL	11-A	1000	-	5,5,5	0.34	0	5,5,5	0.56	0
2	GOL	11-B	1000	-	5,5,5	0.16	0	5,5,5	0.38	0
2	GOL	12-A	1000	-	5,5,5	0.42	0	5,5,5	1.46	1 (20%)
2	GOL	12-B	1000	-	5,5,5	0.15	0	5,5,5	0.38	0
2	GOL	13-A	1000	-	5,5,5	0.73	0	5,5,5	1.00	0
2	GOL	13-B	1000	-	5,5,5	0.14	0	5,5,5	0.40	0
2	GOL	14-A	1000	-	5,5,5	0.26	0	5,5,5	1.58	0
2	GOL	14-B	1000	-	5,5,5	0.20	0	5,5,5	0.48	0
2	GOL	15-A	1000	-	5,5,5	0.41	0	5,5,5	0.67	0
2	GOL	15-B	1000	-	5,5,5	0.16	0	5,5,5	0.40	0
2	GOL	16-A	1000	-	5,5,5	0.28	0	5,5,5	1.48	1 (20%)
2	GOL	16-B	1000	-	5,5,5	0.18	0	5,5,5	0.43	0
2	GOL	17-A	1000	-	5,5,5	0.54	0	5,5,5	1.80	2 (40%)
2	GOL	17-B	1000	-	5,5,5	0.18	0	5,5,5	0.43	0
2	GOL	18-A	1000	-	5,5,5	0.50	0	5,5,5	1.64	1 (20%)
2	GOL	18-B	1000	-	5,5,5	0.17	0	5,5,5	0.40	0
2	GOL	19-A	1000	-	5,5,5	0.41	0	5,5,5	1.64	1 (20%)
2	GOL	19-B	1000	-	5,5,5	0.19	0	5,5,5	0.40	0
2	GOL	2-A	1000	-	5,5,5	0.29	0	5,5,5	1.41	1 (20%)
2	GOL	2-B	1000	-	5,5,5	0.23	0	5,5,5	0.38	0
2	GOL	20-A	1000	-	5,5,5	0.34	0	5,5,5	1.55	1 (20%)
2	GOL	20-B	1000	-	5,5,5	0.21	0	5,5,5	0.37	0
2	GOL	21-A	1000	-	5,5,5	0.53	0	5,5,5	1.84	2 (40%)
2	GOL	21-B	1000	-	5,5,5	0.20	0	5,5,5	0.32	0
2	GOL	22-A	1000	-	5,5,5	0.34	0	5,5,5	1.67	2 (40%)
2	GOL	22-B	1000	-	5,5,5	0.19	0	5,5,5	0.41	0
2	GOL	23-A	1000	-	5,5,5	0.55	0	5,5,5	1.06	0
2	GOL	23-B	1000	-	5,5,5	0.20	0	5,5,5	0.36	0
2	GOL	24-A	1000	-	5,5,5	0.41	0	5,5,5	0.54	0
2	GOL	24-B	1000	-	5,5,5	0.16	0	5,5,5	0.36	0
2	GOL	25-A	1000	-	5,5,5	0.29	0	5,5,5	1.18	0
2	GOL	25-B	1000	-	5,5,5	0.20	0	5,5,5	0.39	0
2	GOL	26-A	1000	-	5,5,5	0.44	0	5,5,5	1.35	0
2	GOL	26-B	1000	-	5,5,5	0.21	0	5,5,5	0.43	0
2	GOL	27-A	1000	-	5,5,5	0.44	0	5,5,5	1.59	1 (20%)
2	GOL	27-B	1000	-	5,5,5	0.24	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	28-A	1000	-	5,5,5	0.47	0	5,5,5	1.73	2 (40%)
2	GOL	28-B	1000	-	5,5,5	0.22	0	5,5,5	0.41	0
2	GOL	29-A	1000	-	5,5,5	0.39	0	5,5,5	1.87	2 (40%)
2	GOL	29-B	1000	-	5,5,5	0.19	0	5,5,5	0.50	0
2	GOL	3-A	1000	-	5,5,5	0.43	0	5,5,5	1.39	0
2	GOL	3-B	1000	-	5,5,5	0.18	0	5,5,5	0.33	0
2	GOL	30-A	1000	-	5,5,5	0.41	0	5,5,5	1.69	1 (20%)
2	GOL	30-B	1000	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	31-A	1000	-	5,5,5	0.88	0	5,5,5	0.99	0
2	GOL	31-B	1000	-	5,5,5	0.20	0	5,5,5	0.37	0
2	GOL	32-A	1000	-	5,5,5	0.27	0	5,5,5	0.27	0
2	GOL	32-B	1000	-	5,5,5	0.22	0	5,5,5	0.37	0
2	GOL	33-A	1000	-	5,5,5	0.57	0	5,5,5	0.82	0
2	GOL	33-B	1000	-	5,5,5	0.19	0	5,5,5	0.35	0
2	GOL	34-A	1000	-	5,5,5	0.56	0	5,5,5	1.47	0
2	GOL	34-B	1000	-	5,5,5	0.27	0	5,5,5	0.31	0
2	GOL	35-A	1000	-	5,5,5	0.55	0	5,5,5	1.62	1 (20%)
2	GOL	35-B	1000	-	5,5,5	0.19	0	5,5,5	0.36	0
2	GOL	36-A	1000	-	5,5,5	0.44	0	5,5,5	1.10	0
2	GOL	36-B	1000	-	5,5,5	0.22	0	5,5,5	0.37	0
2	GOL	37-A	1000	-	5,5,5	0.54	0	5,5,5	1.61	0
2	GOL	37-B	1000	-	5,5,5	0.22	0	5,5,5	0.36	0
2	GOL	38-A	1000	-	5,5,5	0.40	0	5,5,5	1.10	0
2	GOL	38-B	1000	-	5,5,5	0.24	0	5,5,5	0.54	0
2	GOL	39-A	1000	-	5,5,5	0.79	0	5,5,5	0.57	0
2	GOL	39-B	1000	-	5,5,5	0.24	0	5,5,5	0.36	0
2	GOL	4-A	1000	-	5,5,5	0.39	0	5,5,5	1.58	0
2	GOL	4-B	1000	-	5,5,5	0.14	0	5,5,5	0.39	0
2	GOL	40-A	1000	-	5,5,5	0.61	0	5,5,5	0.42	0
2	GOL	40-B	1000	-	5,5,5	0.20	0	5,5,5	0.40	0
2	GOL	41-A	1000	-	5,5,5	0.32	0	5,5,5	1.84	1 (20%)
2	GOL	41-B	1000	-	5,5,5	0.19	0	5,5,5	0.48	0
2	GOL	42-A	1000	-	5,5,5	0.61	0	5,5,5	1.15	0
2	GOL	42-B	1000	-	5,5,5	0.24	0	5,5,5	0.33	0
2	GOL	43-A	1000	-	5,5,5	0.27	0	5,5,5	1.23	0
2	GOL	43-B	1000	-	5,5,5	0.19	0	5,5,5	0.34	0
2	GOL	44-A	1000	-	5,5,5	0.37	0	5,5,5	0.49	0
2	GOL	44-B	1000	-	5,5,5	0.24	0	5,5,5	0.46	0
2	GOL	45-A	1000	-	5,5,5	0.69	0	5,5,5	0.94	0
2	GOL	45-B	1000	-	5,5,5	0.22	0	5,5,5	0.40	0
2	GOL	46-A	1000	-	5,5,5	0.32	0	5,5,5	1.20	0
2	GOL	46-B	1000	-	5,5,5	0.19	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	47-A	1000	-	5,5,5	0.58	0	5,5,5	0.66	0
2	GOL	47-B	1000	-	5,5,5	0.12	0	5,5,5	0.39	0
2	GOL	48-A	1000	-	5,5,5	0.39	0	5,5,5	1.58	1 (20%)
2	GOL	48-B	1000	-	5,5,5	0.17	0	5,5,5	0.51	0
2	GOL	49-A	1000	-	5,5,5	0.42	0	5,5,5	1.87	2 (40%)
2	GOL	49-B	1000	-	5,5,5	0.15	0	5,5,5	0.56	0
2	GOL	5-A	1000	-	5,5,5	0.35	0	5,5,5	1.52	0
2	GOL	5-B	1000	-	5,5,5	0.17	0	5,5,5	0.32	0
2	GOL	50-A	1000	-	5,5,5	0.40	0	5,5,5	1.50	0
2	GOL	50-B	1000	-	5,5,5	0.18	0	5,5,5	0.49	0
2	GOL	51-A	1000	-	5,5,5	0.44	0	5,5,5	1.63	1 (20%)
2	GOL	51-B	1000	-	5,5,5	0.18	0	5,5,5	0.46	0
2	GOL	52-A	1000	-	5,5,5	0.55	0	5,5,5	1.62	1 (20%)
2	GOL	52-B	1000	-	5,5,5	0.19	0	5,5,5	0.54	0
2	GOL	53-A	1000	-	5,5,5	0.33	0	5,5,5	1.56	1 (20%)
2	GOL	53-B	1000	-	5,5,5	0.21	0	5,5,5	0.55	0
2	GOL	54-A	1000	-	5,5,5	0.38	0	5,5,5	1.67	2 (40%)
2	GOL	54-B	1000	-	5,5,5	0.15	0	5,5,5	0.51	0
2	GOL	55-A	1000	-	5,5,5	0.31	0	5,5,5	1.63	1 (20%)
2	GOL	55-B	1000	-	5,5,5	0.18	0	5,5,5	0.43	0
2	GOL	56-A	1000	-	5,5,5	0.42	0	5,5,5	0.52	0
2	GOL	56-B	1000	-	5,5,5	0.20	0	5,5,5	0.45	0
2	GOL	57-A	1000	-	5,5,5	0.32	0	5,5,5	1.16	0
2	GOL	57-B	1000	-	5,5,5	0.21	0	5,5,5	0.44	0
2	GOL	58-A	1000	-	5,5,5	0.41	0	5,5,5	1.58	1 (20%)
2	GOL	58-B	1000	-	5,5,5	0.16	0	5,5,5	0.52	0
2	GOL	59-A	1000	-	5,5,5	0.33	0	5,5,5	1.44	0
2	GOL	59-B	1000	-	5,5,5	0.14	0	5,5,5	0.49	0
2	GOL	6-A	1000	-	5,5,5	0.34	0	5,5,5	1.42	0
2	GOL	6-B	1000	-	5,5,5	0.16	0	5,5,5	0.30	0
2	GOL	60-A	1000	-	5,5,5	0.44	0	5,5,5	1.05	0
2	GOL	60-B	1000	-	5,5,5	0.18	0	5,5,5	0.46	0
2	GOL	61-A	1000	-	5,5,5	0.36	0	5,5,5	1.14	0
2	GOL	61-B	1000	-	5,5,5	0.19	0	5,5,5	0.52	0
2	GOL	62-A	1000	-	5,5,5	0.45	0	5,5,5	0.38	0
2	GOL	62-B	1000	-	5,5,5	0.17	0	5,5,5	0.45	0
2	GOL	63-A	1000	-	5,5,5	0.40	0	5,5,5	0.35	0
2	GOL	63-B	1000	-	5,5,5	0.13	0	5,5,5	0.45	0
2	GOL	64-A	1000	-	5,5,5	0.63	0	5,5,5	1.89	1 (20%)
2	GOL	64-B	1000	-	5,5,5	0.12	0	5,5,5	0.48	0
2	GOL	65-A	1000	-	5,5,5	0.46	0	5,5,5	1.59	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	65-B	1000	-	5,5,5	0.13	0	5,5,5	0.59	0
2	GOL	66-A	1000	-	5,5,5	0.46	0	5,5,5	1.23	1 (20%)
2	GOL	66-B	1000	-	5,5,5	0.11	0	5,5,5	0.57	0
2	GOL	67-A	1000	-	5,5,5	0.53	0	5,5,5	0.28	0
2	GOL	67-B	1000	-	5,5,5	0.12	0	5,5,5	0.48	0
2	GOL	68-A	1000	-	5,5,5	0.45	0	5,5,5	1.39	0
2	GOL	68-B	1000	-	5,5,5	0.11	0	5,5,5	0.47	0
2	GOL	69-A	1000	-	5,5,5	0.28	0	5,5,5	1.13	0
2	GOL	69-B	1000	-	5,5,5	0.14	0	5,5,5	0.48	0
2	GOL	7-A	1000	-	5,5,5	0.34	0	5,5,5	1.58	0
2	GOL	7-B	1000	-	5,5,5	0.20	0	5,5,5	0.31	0
2	GOL	70-A	1000	-	5,5,5	0.31	0	5,5,5	0.76	0
2	GOL	70-B	1000	-	5,5,5	0.15	0	5,5,5	0.50	0
2	GOL	71-A	1000	-	5,5,5	0.40	0	5,5,5	1.34	0
2	GOL	71-B	1000	-	5,5,5	0.21	0	5,5,5	0.56	0
2	GOL	72-A	1000	-	5,5,5	0.38	0	5,5,5	1.55	0
2	GOL	72-B	1000	-	5,5,5	0.18	0	5,5,5	0.43	0
2	GOL	73-A	1000	-	5,5,5	0.31	0	5,5,5	1.40	0
2	GOL	73-B	1000	-	5,5,5	0.20	0	5,5,5	0.55	0
2	GOL	74-A	1000	-	5,5,5	0.36	0	5,5,5	1.64	1 (20%)
2	GOL	74-B	1000	-	5,5,5	0.20	0	5,5,5	0.52	0
2	GOL	75-A	1000	-	5,5,5	0.36	0	5,5,5	1.56	1 (20%)
2	GOL	75-B	1000	-	5,5,5	0.19	0	5,5,5	0.57	0
2	GOL	76-A	1000	-	5,5,5	0.47	0	5,5,5	1.53	1 (20%)
2	GOL	76-B	1000	-	5,5,5	0.15	0	5,5,5	0.62	0
2	GOL	77-A	1000	-	5,5,5	0.46	0	5,5,5	1.24	0
2	GOL	77-B	1000	-	5,5,5	0.17	0	5,5,5	0.50	0
2	GOL	8-A	1000	-	5,5,5	0.28	0	5,5,5	1.42	0
2	GOL	8-B	1000	-	5,5,5	0.17	0	5,5,5	0.41	0
2	GOL	9-A	1000	-	5,5,5	0.33	0	5,5,5	0.54	0
2	GOL	9-B	1000	-	5,5,5	0.19	0	5,5,5	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	1-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	1-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	10-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	10-B	1000	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	11-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	11-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	12-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	12-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	13-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	13-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	14-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	14-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	15-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	15-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	16-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	16-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	17-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	17-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	18-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	18-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	19-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	19-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	2-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	2-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	20-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	20-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	21-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	21-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	22-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	22-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	23-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	23-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	24-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	24-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	25-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	25-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	26-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	26-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	27-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	27-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	28-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	28-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	29-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	29-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	3-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	3-B	1000	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	30-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	30-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	31-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	31-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	32-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	32-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	33-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	33-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	34-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	34-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	35-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	35-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	36-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	36-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	37-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	37-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	38-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	38-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	39-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	39-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	4-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	4-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	40-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	40-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	41-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	41-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	42-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	42-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	43-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	43-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	44-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	44-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	45-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	45-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	46-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	46-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	47-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	47-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	48-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	48-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	49-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	49-B	1000	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	5-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	5-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	50-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	50-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	51-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	51-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	52-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	52-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	53-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	53-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	54-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	54-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	55-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	55-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	56-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	56-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	57-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	57-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	58-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	58-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	59-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	59-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	6-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	6-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	60-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	60-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	61-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	61-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	62-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	62-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	63-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	63-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	64-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	64-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	65-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	65-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	66-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	66-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	67-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	67-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	68-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	68-B	1000	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	69-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	69-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	7-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	7-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	70-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	70-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	71-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	71-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	72-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	72-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	73-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	73-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	74-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	74-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	75-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	75-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	76-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	76-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	77-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	77-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	8-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	8-B	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	9-A	1000	-	-	0/4/4/4	0/0/0/0
2	GOL	9-B	1000	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	64-A	1000	GOL	O1-C1-C2	3.16	124.39	110.37
2	41-A	1000	GOL	O2-C2-C1	-2.87	95.16	108.44
2	49-A	1000	GOL	O2-C2-C1	2.85	121.66	108.44
2	48-A	1000	GOL	O2-C2-C1	-2.54	96.67	108.44
2	16-A	1000	GOL	O2-C2-C1	-2.48	96.95	108.44

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	1-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	2-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	2-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	3-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	3-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	4-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	4-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	5-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	5-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	6-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	6-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	7-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	7-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	8-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	8-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	9-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	9-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	10-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	10-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	11-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	11-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	12-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	12-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	13-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	13-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	14-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	14-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	15-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	15-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	16-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	16-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	17-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	17-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	18-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	18-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	19-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	19-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	20-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	20-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	21-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	21-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	22-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	22-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	23-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	23-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	24-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	24-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	25-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	25-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	26-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	26-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	27-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	27-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	28-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	28-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	29-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	29-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	30-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	30-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	31-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	31-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	32-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	32-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	33-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	33-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	34-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	34-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	35-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	35-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	36-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	36-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	37-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	37-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	38-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	38-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	39-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	39-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	40-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	40-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	41-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	41-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	42-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	42-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	43-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	43-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	44-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	44-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	45-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	45-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	46-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	46-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	47-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	47-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	48-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	48-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	49-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	49-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	50-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	50-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	51-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	51-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	52-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	52-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	53-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	53-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	54-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	54-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	55-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	55-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	56-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	56-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	57-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	57-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	58-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)
1	58-B	228/228 (100%)	0.63	22 (9%)	8	6	16, 27, 46, 61	228 (100%)
1	59-A	228/228 (100%)	1.50	45 (19%)	2	1	14, 23, 40, 46	228 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	59-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	60-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	60-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	61-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	61-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	62-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	62-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	63-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	63-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	64-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	64-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	65-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	65-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	66-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	66-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	67-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	67-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	68-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	68-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	69-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	69-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	70-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	70-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	71-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	71-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	72-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	72-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	73-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	73-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	74-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	74-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	75-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	75-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	76-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	76-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
1	77-A	228/228 (100%)	1.50	45 (19%) 2 1	14, 23, 40, 46	228 (100%)
1	77-B	228/228 (100%)	0.63	22 (9%) 8 6	16, 27, 46, 61	228 (100%)
All	All	35112/35112 (100%)	1.07	5159 (14%) 3 2	14, 25, 42, 61	35112 (100%)

The worst 5 of 5159 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	131	VAL	39.2
1	2-A	131	VAL	39.2
1	3-A	131	VAL	39.2
1	4-A	131	VAL	39.2
1	5-A	131	VAL	39.2

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, 95th 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 ²)	Q<0.9
2	GOL	45-A	1000	6/6	0.12	0.95	18,19,20,21	14
2	GOL	36-A	1000	6/6	0.12	0.89	18,19,20,21	14
2	GOL	77-A	1000	6/6	0.12	0.88	18,19,20,21	14

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	13-A	1000	6/6	0.12	0.87	18,19,21,21	14
2	GOL	60-A	1000	6/6	0.12	0.85	18,19,20,20	14
2	GOL	47-A	1000	6/6	0.12	0.82	18,19,20,21	14
2	GOL	68-A	1000	6/6	0.12	0.81	18,19,21,21	14
2	GOL	23-A	1000	6/6	0.12	0.81	18,19,20,20	14
2	GOL	38-A	1000	6/6	0.12	0.81	18,19,20,20	14
2	GOL	42-A	1000	6/6	0.12	0.81	18,19,20,21	14
2	GOL	44-A	1000	6/6	0.12	0.72	18,19,21,21	14
2	GOL	32-A	1000	6/6	0.12	0.72	18,19,20,21	14
2	GOL	15-A	1000	6/6	0.12	0.66	18,19,20,21	14
2	GOL	56-A	1000	6/6	0.12	0.65	18,19,20,21	14
2	GOL	70-A	1000	6/6	0.12	0.63	18,19,21,21	14
2	GOL	68-B	1000	6/6	0.19	0.60	30,32,37,38	14
2	GOL	26-A	1000	6/6	0.12	0.60	18,19,20,21	14
2	GOL	24-A	1000	6/6	0.12	0.60	18,19,21,21	14
2	GOL	63-B	1000	6/6	0.19	0.60	30,32,37,38	14
2	GOL	11-B	1000	6/6	0.19	0.60	30,33,37,38	14
2	GOL	31-B	1000	6/6	0.19	0.60	30,32,36,38	14
2	GOL	12-B	1000	6/6	0.19	0.60	30,33,37,38	14
2	GOL	69-B	1000	6/6	0.19	0.60	30,32,37,38	14
2	GOL	20-A	1000	6/6	0.12	0.60	18,19,20,21	14
2	GOL	24-B	1000	6/6	0.19	0.60	30,32,36,38	14
2	GOL	66-A	1000	6/6	0.12	0.60	18,19,20,21	14
2	GOL	72-B	1000	6/6	0.19	0.60	31,33,37,38	14
2	GOL	61-A	1000	6/6	0.12	0.60	18,19,20,21	14
2	GOL	62-B	1000	6/6	0.19	0.60	30,32,36,38	14
2	GOL	33-B	1000	6/6	0.19	0.60	30,32,37,38	14
2	GOL	32-B	1000	6/6	0.19	0.60	30,32,37,38	14
2	GOL	27-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	13-B	1000	6/6	0.19	0.59	30,32,36,38	14
2	GOL	67-B	1000	6/6	0.19	0.59	30,32,37,38	14
2	GOL	17-B	1000	6/6	0.19	0.59	31,32,37,38	14
2	GOL	59-B	1000	6/6	0.19	0.59	30,33,37,38	14
2	GOL	66-B	1000	6/6	0.19	0.59	30,33,37,38	14
2	GOL	22-B	1000	6/6	0.19	0.59	31,32,37,38	14
2	GOL	64-A	1000	6/6	0.12	0.59	18,19,20,20	14
2	GOL	76-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	35-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	35-B	1000	6/6	0.19	0.59	30,33,37,38	14
2	GOL	18-B	1000	6/6	0.19	0.59	31,32,37,38	14
2	GOL	28-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	10-A	1000	6/6	0.12	0.59	18,19,21,21	14

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	64-B	1000	6/6	0.19	0.59	30,32,36,38	14
2	GOL	75-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	41-A	1000	6/6	0.12	0.59	18,19,20,20	14
2	GOL	34-B	1000	6/6	0.19	0.59	30,32,36,38	14
2	GOL	39-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	36-B	1000	6/6	0.19	0.59	30,32,37,38	14
2	GOL	70-B	1000	6/6	0.19	0.59	30,32,37,38	14
2	GOL	26-B	1000	6/6	0.19	0.59	30,32,37,38	14
2	GOL	25-A	1000	6/6	0.12	0.59	18,19,21,21	14
2	GOL	57-A	1000	6/6	0.12	0.59	18,19,20,21	14
2	GOL	19-B	1000	6/6	0.19	0.58	30,32,36,38	14
2	GOL	67-A	1000	6/6	0.12	0.58	18,19,21,21	14
2	GOL	77-B	1000	6/6	0.19	0.58	30,33,37,38	14
2	GOL	27-B	1000	6/6	0.19	0.58	30,32,36,38	14
2	GOL	73-A	1000	6/6	0.12	0.58	18,19,20,20	14
2	GOL	59-A	1000	6/6	0.12	0.58	18,19,20,20	14
2	GOL	10-B	1000	6/6	0.19	0.58	30,32,37,38	14
2	GOL	16-B	1000	6/6	0.19	0.58	30,32,37,38	14
2	GOL	15-B	1000	6/6	0.19	0.58	30,32,36,38	14
2	GOL	71-B	1000	6/6	0.19	0.58	31,33,37,38	14
2	GOL	65-B	1000	6/6	0.19	0.58	30,32,36,38	14
2	GOL	11-A	1000	6/6	0.12	0.58	18,19,20,21	14
2	GOL	21-B	1000	6/6	0.19	0.57	30,32,37,38	14
2	GOL	62-A	1000	6/6	0.12	0.57	18,19,21,21	14
2	GOL	48-A	1000	6/6	0.12	0.57	18,19,20,21	14
2	GOL	23-B	1000	6/6	0.19	0.57	30,32,37,38	14
2	GOL	14-A	1000	6/6	0.12	0.57	18,19,21,21	14
2	GOL	73-B	1000	6/6	0.19	0.57	30,32,37,38	14
2	GOL	37-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	76-B	1000	6/6	0.19	0.56	30,33,37,38	14
2	GOL	25-B	1000	6/6	0.19	0.56	30,32,37,38	14
2	GOL	16-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	17-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	61-B	1000	6/6	0.19	0.56	30,32,37,38	14
2	GOL	65-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	20-B	1000	6/6	0.19	0.56	30,32,37,38	14
2	GOL	30-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	49-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	14-B	1000	6/6	0.19	0.56	30,32,36,38	14
2	GOL	72-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	29-B	1000	6/6	0.19	0.56	30,33,37,38	14
2	GOL	69-A	1000	6/6	0.12	0.56	18,19,20,20	14

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	22-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	55-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	29-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	55-B	1000	6/6	0.19	0.56	29,32,36,38	14
2	GOL	19-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	74-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	28-B	1000	6/6	0.19	0.56	30,32,37,38	14
2	GOL	58-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	40-A	1000	6/6	0.12	0.56	18,19,21,21	14
2	GOL	37-B	1000	6/6	0.19	0.56	30,32,37,38	14
2	GOL	50-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	18-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	54-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	51-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	52-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	74-B	1000	6/6	0.19	0.56	30,33,37,38	14
2	GOL	53-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	71-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	21-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	60-B	1000	6/6	0.19	0.56	30,33,37,38	14
2	GOL	12-A	1000	6/6	0.12	0.56	18,19,20,21	14
2	GOL	63-A	1000	6/6	0.12	0.56	18,19,21,21	14
2	GOL	34-A	1000	6/6	0.12	0.56	18,19,20,20	14
2	GOL	33-A	1000	6/6	0.12	0.55	18,19,21,21	14
2	GOL	46-A	1000	6/6	0.12	0.55	18,19,21,21	14
2	GOL	58-B	1000	6/6	0.19	0.55	29,32,37,38	14
2	GOL	31-A	1000	6/6	0.12	0.55	18,19,20,21	14
2	GOL	38-B	1000	6/6	0.19	0.55	29,32,36,38	14
2	GOL	43-A	1000	6/6	0.12	0.55	18,19,20,21	14
2	GOL	30-B	1000	6/6	0.19	0.54	30,33,37,38	14
2	GOL	75-B	1000	6/6	0.19	0.54	30,32,37,38	14
2	GOL	56-B	1000	6/6	0.19	0.53	29,32,37,38	14
2	GOL	50-B	1000	6/6	0.19	0.53	29,32,37,38	14
2	GOL	40-B	1000	6/6	0.19	0.53	29,32,37,38	14
2	GOL	51-B	1000	6/6	0.19	0.53	29,33,37,38	14
2	GOL	54-B	1000	6/6	0.19	0.52	29,32,36,38	14
2	GOL	49-B	1000	6/6	0.19	0.52	29,32,36,38	14
2	GOL	43-B	1000	6/6	0.19	0.52	29,32,37,38	14
2	GOL	46-B	1000	6/6	0.19	0.52	29,32,36,38	14
2	GOL	57-B	1000	6/6	0.19	0.52	29,32,36,38	14
2	GOL	41-B	1000	6/6	0.19	0.51	29,32,36,38	14
2	GOL	52-B	1000	6/6	0.19	0.51	29,32,36,38	14

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	39-B	1000	6/6	0.19	0.51	29,32,36,38	14
2	GOL	47-B	1000	6/6	0.19	0.51	29,32,36,38	14
2	GOL	42-B	1000	6/6	0.19	0.50	29,32,37,38	14
2	GOL	53-B	1000	6/6	0.19	0.50	29,32,37,38	14
2	GOL	48-B	1000	6/6	0.19	0.50	29,32,37,38	14
2	GOL	44-B	1000	6/6	0.19	0.50	29,32,36,38	14
2	GOL	45-B	1000	6/6	0.19	0.48	29,32,36,38	14
2	GOL	4-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	5-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	4-B	1000	6/6	0.19	-	31,33,37,38	14
2	GOL	6-B	1000	6/6	0.19	-	30,32,36,38	14
2	GOL	2-B	1000	6/6	0.19	-	30,32,36,38	14
2	GOL	3-B	1000	6/6	0.19	-	31,32,37,38	14
2	GOL	9-B	1000	6/6	0.19	-	30,32,37,38	14
2	GOL	3-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	6-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	8-B	1000	6/6	0.19	-	30,32,37,38	14
2	GOL	1-B	1000	6/6	0.19	-	30,32,36,38	14
2	GOL	2-A	1000	6/6	0.12	-	18,19,21,21	14
2	GOL	5-B	1000	6/6	0.19	-	31,32,37,38	14
2	GOL	8-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	7-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	1-A	1000	6/6	0.12	-	18,19,20,21	14
2	GOL	9-A	1000	6/6	0.12	-	18,19,21,21	14
2	GOL	7-B	1000	6/6	0.19	-	30,32,37,38	14

6.5 Other polymers ⓘ

There are no such residues in this entry.