



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2018 – 06:49 PM EST

PDB ID : 4R4N
Title : Crystal structure of the anti-hiv-1 antibody 2.2c in complex with hiv-1 93ug037 gp120
Authors : Acharya, P.; Louder, R.; Kwong, P.D.
Deposited on : 2014-08-19
Resolution : 3.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

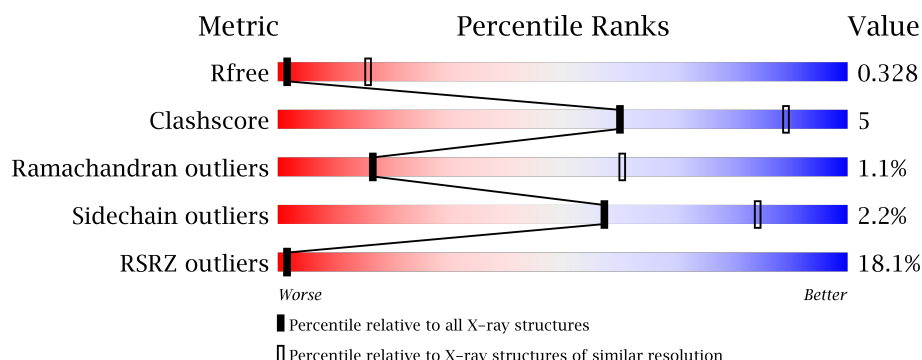
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 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}	100719	1072 (3.70-3.42)
Clashscore	112137	1003 (3.66-3.46)
Ramachandran outliers	110173	1153 (3.70-3.42)
Sidechain outliers	110143	1153 (3.70-3.42)
RSRZ outliers	101464	1098 (3.70-3.42)

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

Mol	Chain	Length	Quality of chain
1	A	352	
1	B	352	
1	E	352	
1	I	352	
1	M	352	

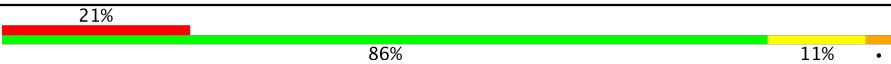
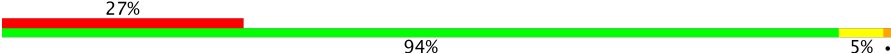
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Mol	Chain	Length	Quality of chain
1	P	352	<div> <div>9%</div> <div>88%</div> <div>7%</div> </div>
1	S	352	<div> <div>7%</div> <div>86%</div> <div>10%</div> </div>
1	V	352	<div> <div>9%</div> <div>88%</div> <div>8%</div> </div>
2	a	28	<div> <div>7%</div> <div>96%</div> </div>
2	b	28	<div> <div>4%</div> <div>100%</div> </div>
2	e	28	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
2	i	28	<div> <div>4%</div> <div>100%</div> </div>
2	m	28	<div> <div>7%</div> <div>100%</div> </div>
2	p	28	<div> <div>7%</div> <div>100%</div> </div>
2	s	28	<div> <div>7%</div> <div>96%</div> </div>
2	v	28	<div> <div>14%</div> <div>100%</div> </div>
3	D	210	<div> <div>25%</div> <div>86%</div> <div>14%</div> </div>
3	G	210	<div> <div>24%</div> <div>93%</div> <div>6%</div> </div>
3	K	210	<div> <div>40%</div> <div>90%</div> <div>9%</div> </div>
3	L	210	<div> <div>14%</div> <div>97%</div> </div>
3	O	210	<div> <div>26%</div> <div>94%</div> <div>6%</div> </div>
3	R	210	<div> <div>24%</div> <div>98%</div> </div>
3	U	210	<div> <div>16%</div> <div>94%</div> <div>6%</div> </div>
3	X	210	<div> <div>32%</div> <div>96%</div> </div>
4	C	220	<div> <div>23%</div> <div>83%</div> <div>13%</div> </div>
4	F	220	<div> <div>24%</div> <div>86%</div> <div>11%</div> </div>
4	H	220	<div> <div>19%</div> <div>95%</div> </div>
4	J	220	<div> <div>35%</div> <div>83%</div> <div>15%</div> </div>
4	N	220	<div> <div>26%</div> <div>86%</div> <div>13%</div> </div>
4	Q	220	<div> <div>21%</div> <div>94%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
4	T	220	
4	W	220	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	502	-	-	X	-
5	NAG	I	502	-	-	-	X
5	NAG	M	501	-	-	-	X
5	NAG	S	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 94738 atoms, of which 45586 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 gp120.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	333	Total	C	H	N	O	S	0	0	0
			5094	1611	2506	458	498	21			
1	B	342	Total	C	H	N	O	S	0	0	0
			5189	1655	2532	469	512	21			
1	I	341	Total	C	H	N	O	S	0	0	0
			5172	1641	2532	466	512	21			
1	E	329	Total	C	H	N	O	S	0	0	0
			5042	1595	2481	453	492	21			
1	M	339	Total	C	H	N	O	S	0	0	0
			5169	1633	2544	463	508	21			
1	P	338	Total	C	H	N	O	S	0	0	0
			5157	1631	2537	462	506	21			
1	S	339	Total	C	H	N	O	S	0	0	0
			5168	1634	2542	463	508	21			
1	V	338	Total	C	H	N	O	S	0	0	0
			5160	1631	2539	463	506	21			

- Molecule 2 is a protein called M48U1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	b	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	e	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	i	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	m	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	p	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	s	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			
2	v	28	Total	C	N	O	S	0	0	1
			209	133	38	32	6			

- Molecule 3 is a protein called Antibody 2.2c LIGHT CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	210	Total 3197	C 1012	H 1585	N 272	O 323	S 5	0	0	0
3	D	210	Total 3196	C 1012	H 1584	N 272	O 323	S 5	0	0	0
3	G	210	Total 3194	C 1012	H 1582	N 272	O 323	S 5	0	0	0
3	K	210	Total 3195	C 1012	H 1583	N 272	O 323	S 5	0	0	0
3	O	210	Total 3198	C 1012	H 1586	N 272	O 323	S 5	0	0	0
3	R	210	Total 3195	C 1012	H 1583	N 272	O 323	S 5	0	0	0
3	U	210	Total 3193	C 1012	H 1581	N 272	O 323	S 5	0	0	0
3	X	210	Total 3198	C 1012	H 1586	N 272	O 323	S 5	0	0	0

- Molecule 4 is a protein called Antibody 2.2c heavy CHAIN.

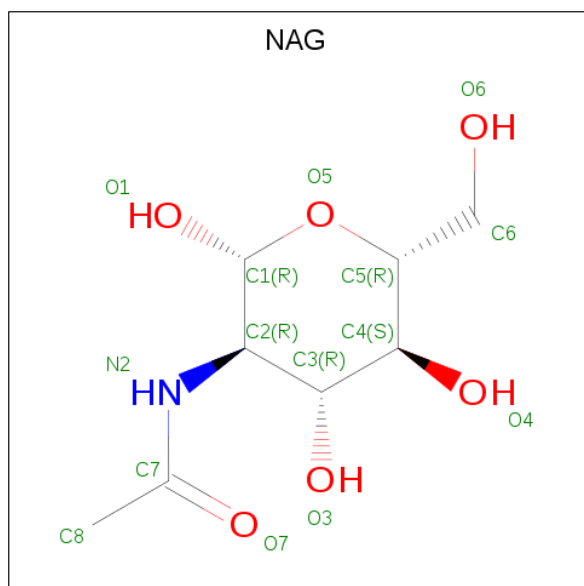
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	220	Total 3322	C 1066	H 1648	N 283	O 320	S 5	0	0	0
4	C	220	Total 3245	C 1066	H 1571	N 283	O 320	S 5	0	0	0
4	F	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	J	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	N	220	Total 3322	C 1064	H 1651	N 283	O 319	S 5	0	0	0
4	Q	220	Total 3322	C 1064	H 1651	N 283	O 319	S 5	0	0	0
4	T	220	Total 3179	C 1066	H 1505	N 283	O 320	S 5	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
4	W	220	Total	C	H	N	O	S	0	0	0
			3321	1066	1647	283	320	5			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	A	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0
5	B	1	Total 14	8	1	5	0	0
5	I	1	Total 14	8	1	5	0	0
5	I	1	Total 14	8	1	5	0	0
5	I	1	Total 14	8	1	5	0	0
5	I	1	Total 14	8	1	5	0	0

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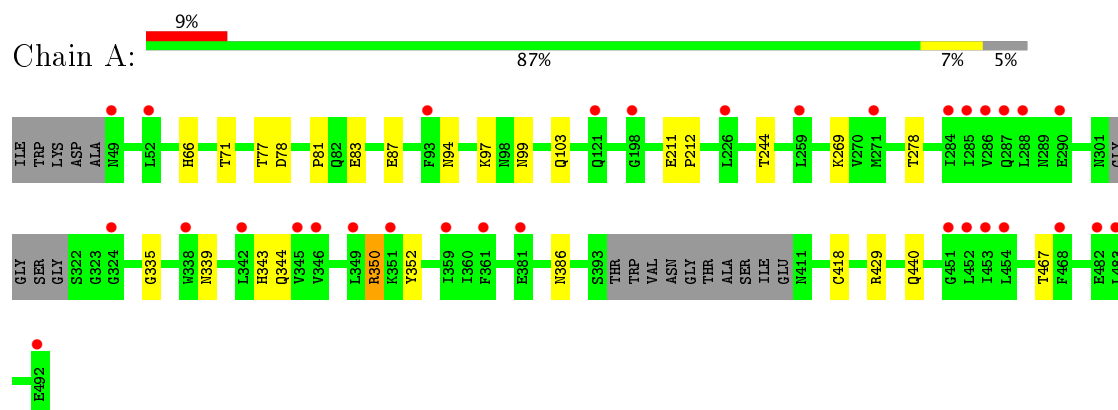
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	S	1	Total	C	N	O	0	0
			14	8	1	5		
5	V	1	Total	C	N	O	0	0
			14	8	1	5		

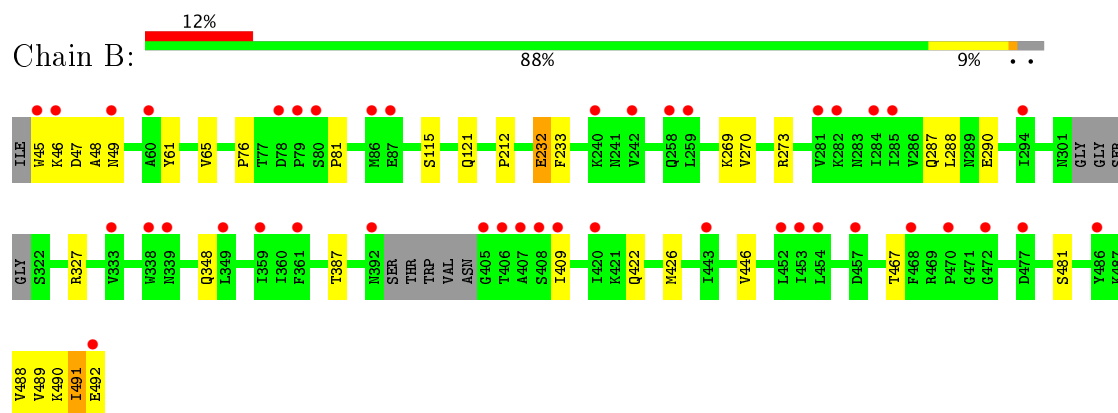
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

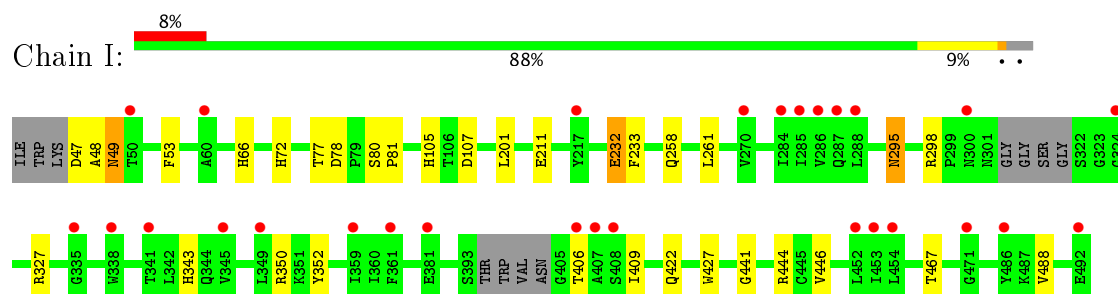
• Molecule 1: HIV-1 gp120



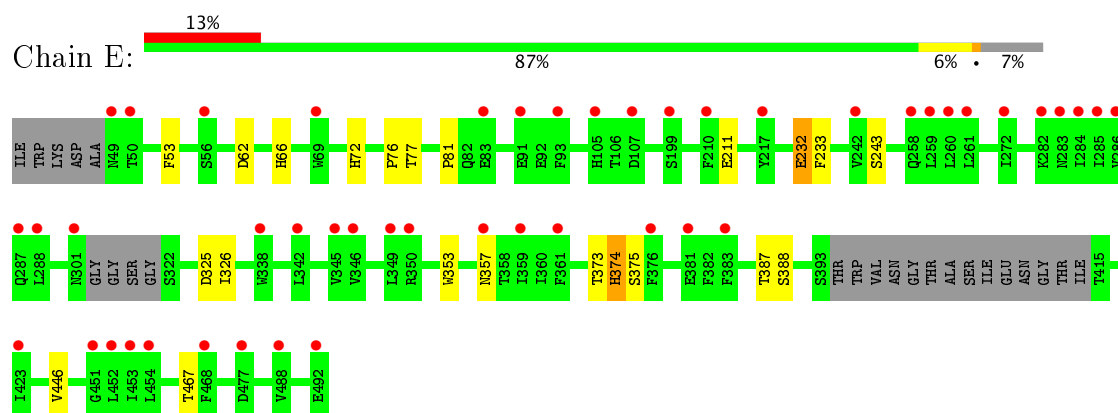
• Molecule 1: HIV-1 gp120



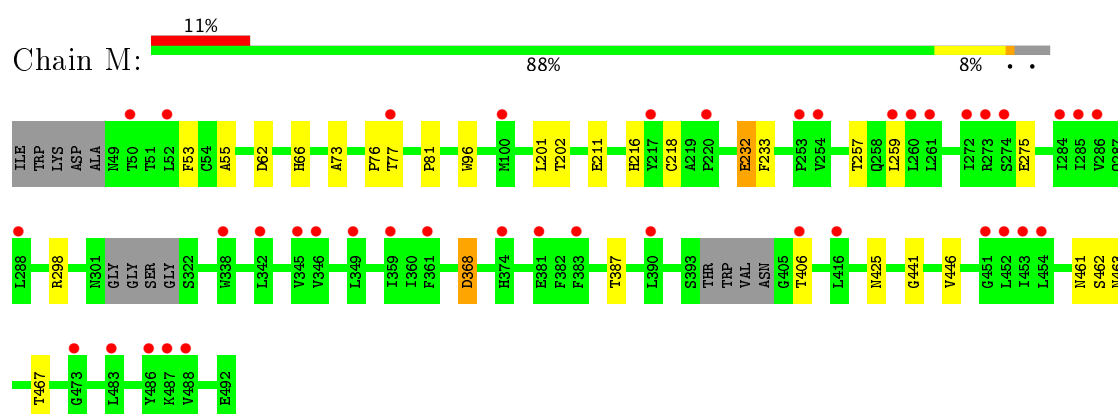
• Molecule 1: HIV-1 gp120



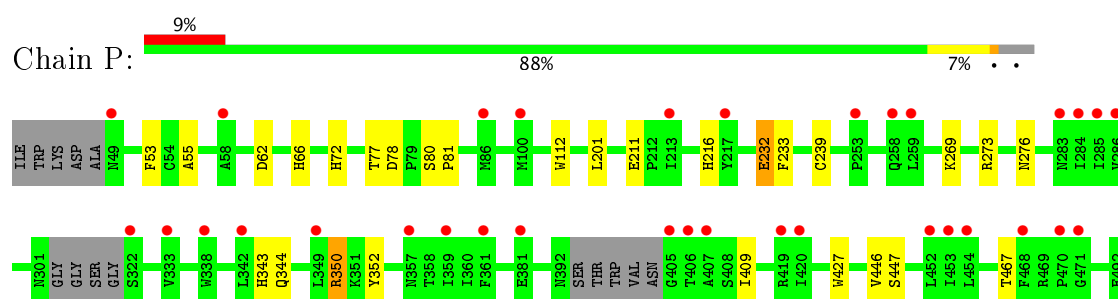
- Molecule 1: HIV-1 gp120



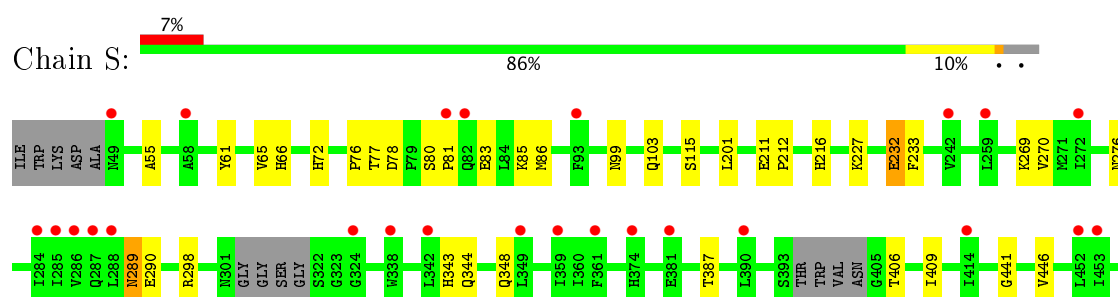
- Molecule 1: HIV-1 gp120



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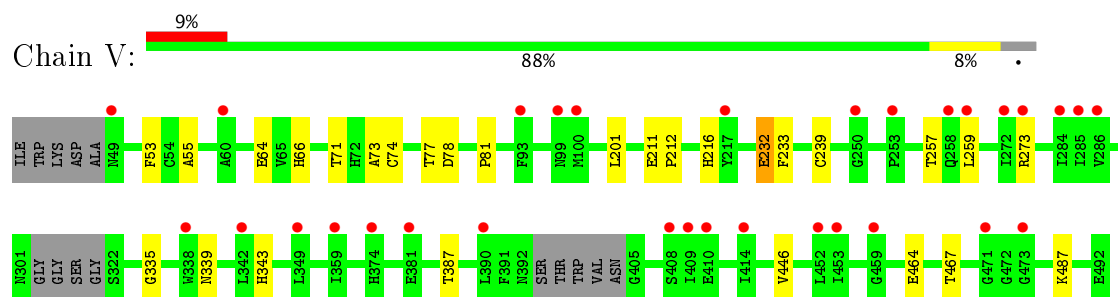


- Molecule 1: HIV-1 gp120

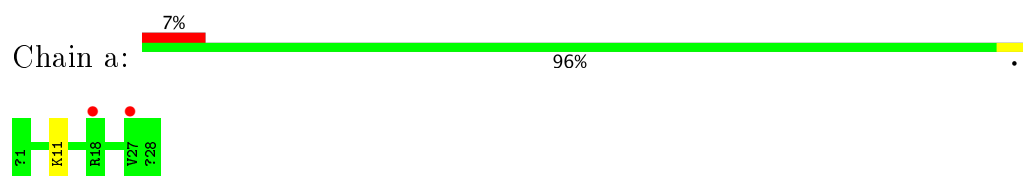




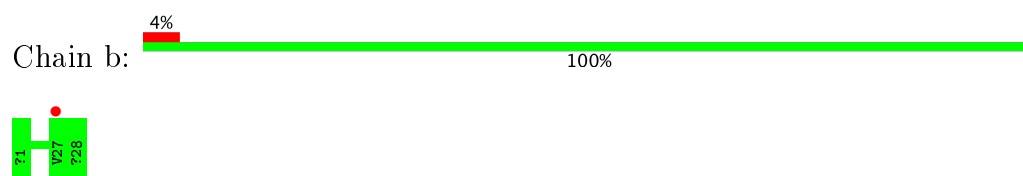
- Molecule 1: HIV-1 gp120



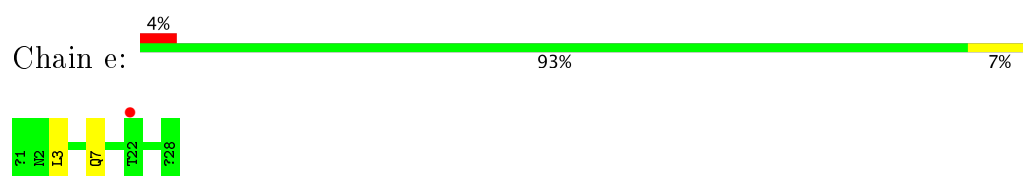
- Molecule 2: M48U1 peptide



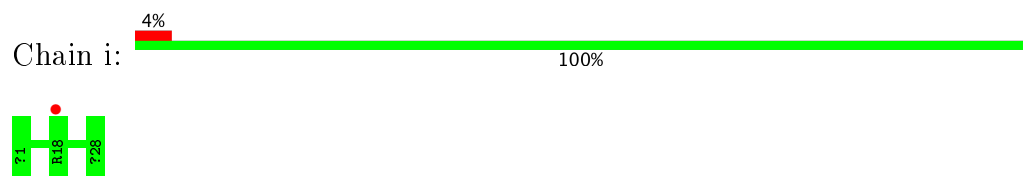
- Molecule 2: M48U1 peptide



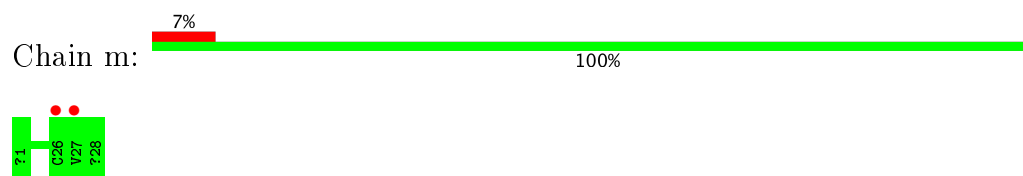
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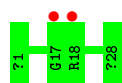
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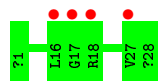
- Molecule 2: M48U1 peptide



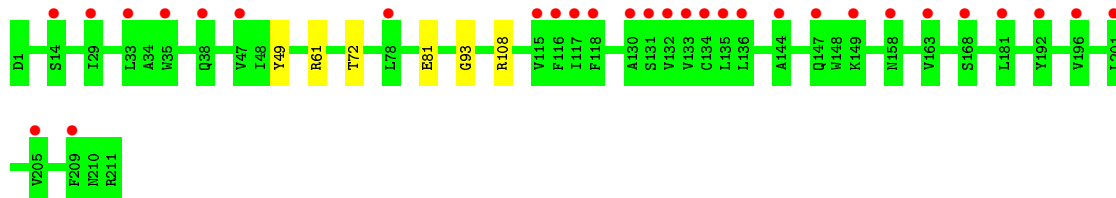
- Molecule 2: M48U1 peptide



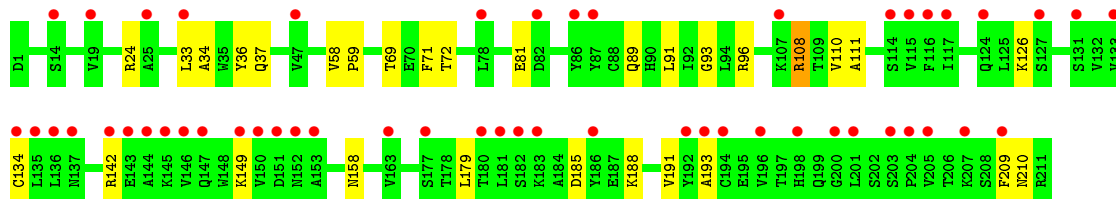
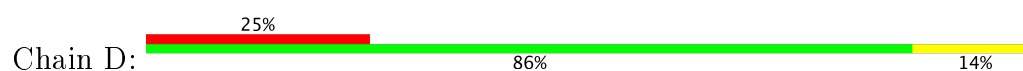
- Molecule 2: M48U1 peptide



- Molecule 3: Antibody 2.2c LIGHT CHAIN

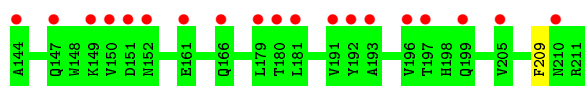


- Molecule 3: Antibody 2.2c LIGHT CHAIN

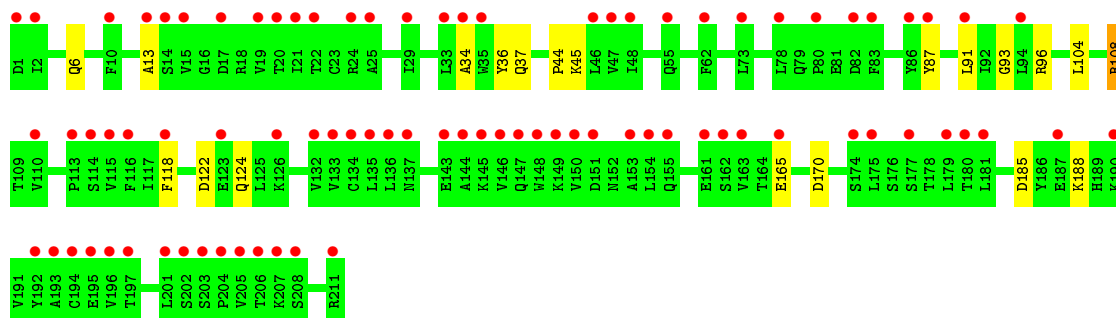
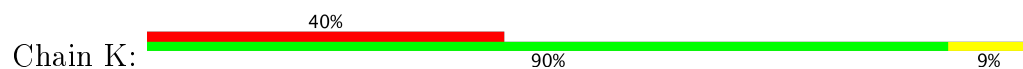


- Molecule 3: Antibody 2.2c LIGHT CHAIN

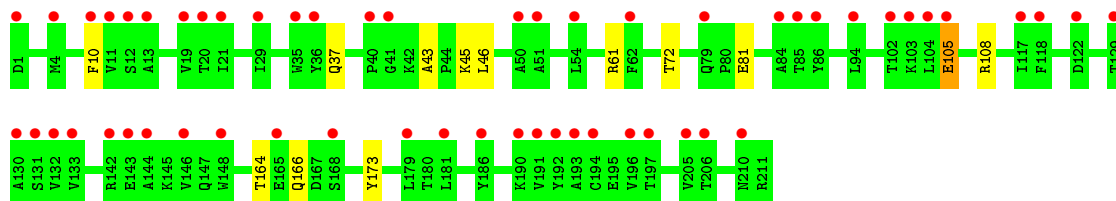




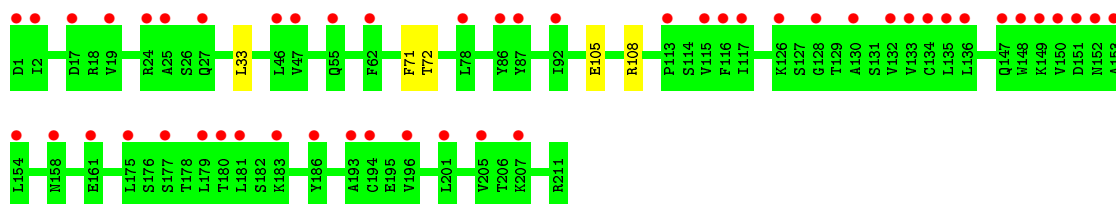
• Molecule 3: Antibody 2.2c LIGHT CHAIN



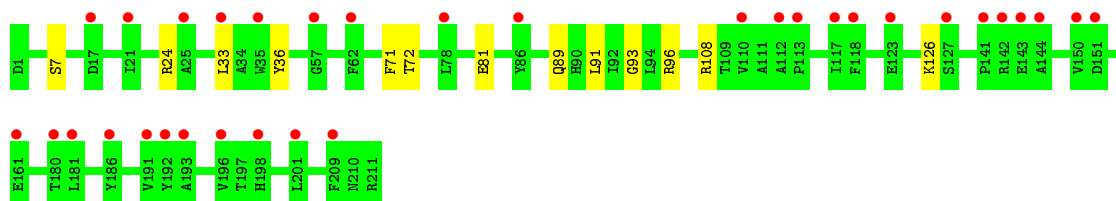
• Molecule 3: Antibody 2.2c LIGHT CHAIN



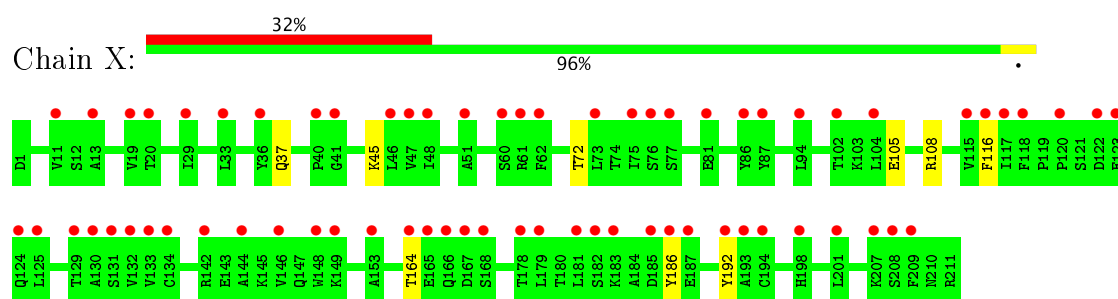
• Molecule 3: Antibody 2.2c LIGHT CHAIN



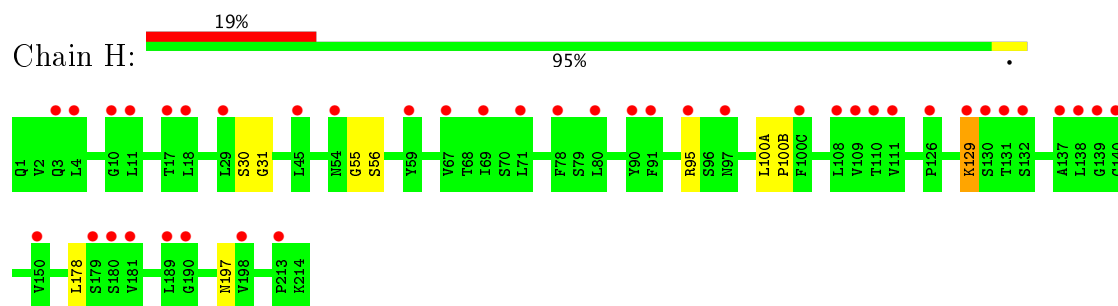
• Molecule 3: Antibody 2.2c LIGHT CHAIN



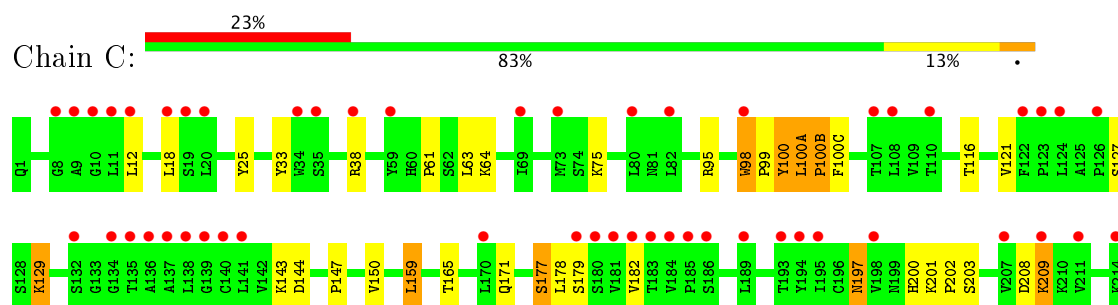
• Molecule 3: Antibody 2.2c LIGHT CHAIN



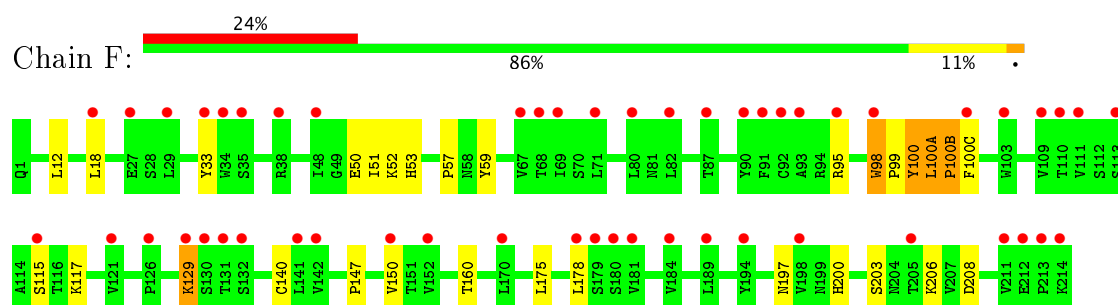
• Molecule 4: Antibody 2.2c heavy CHAIN



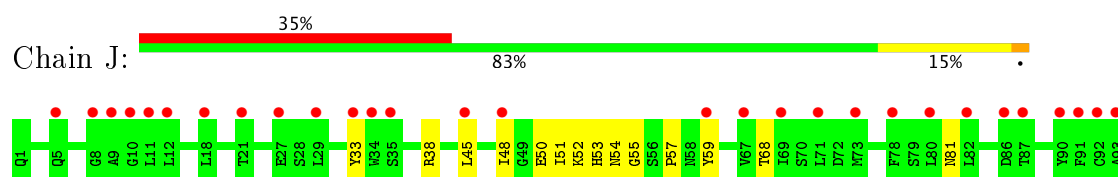
• Molecule 4: Antibody 2.2c heavy CHAIN

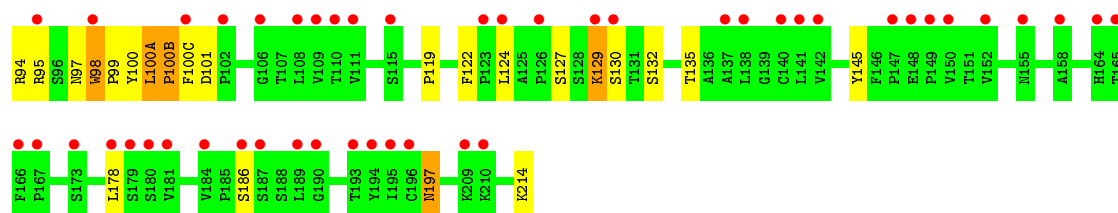


• Molecule 4: Antibody 2.2c heavy CHAIN

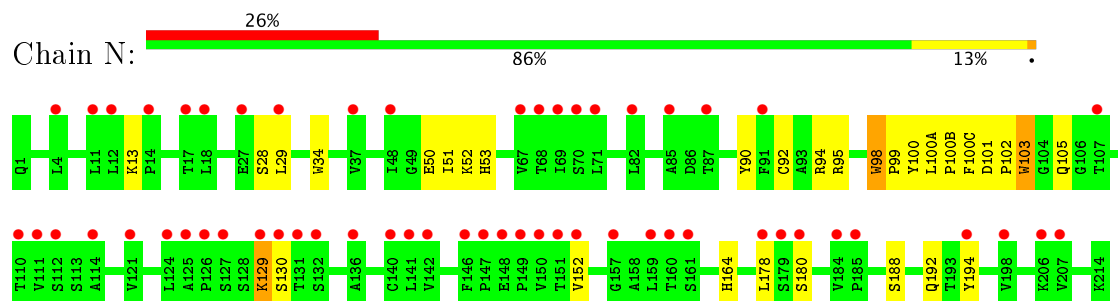


• Molecule 4: Antibody 2.2c heavy CHAIN

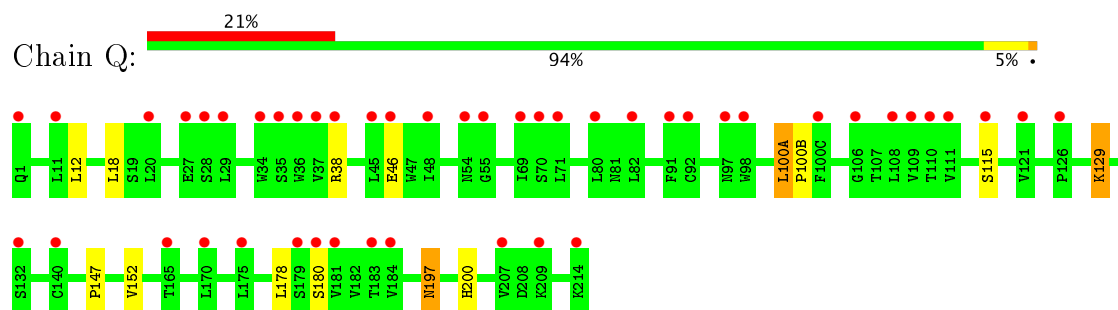




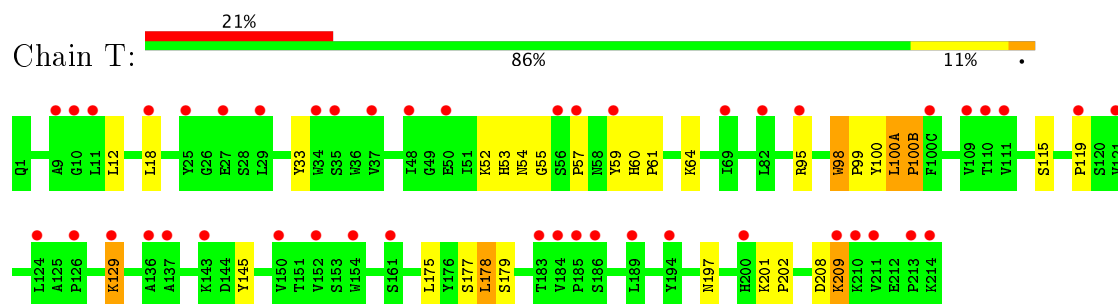
• Molecule 4: Antibody 2.2c heavy CHAIN



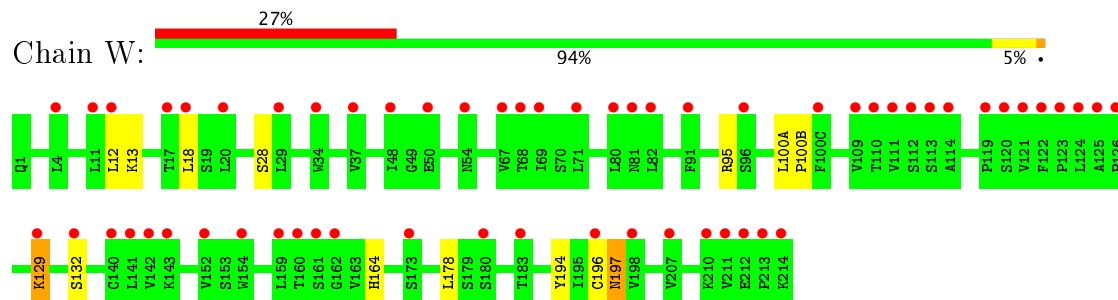
• Molecule 4: Antibody 2.2c heavy CHAIN



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• Molecule 4: Antibody 2.2c heavy CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	112.97Å 144.18Å 158.35Å 110.58° 92.30° 99.19°	Depositor
Resolution (Å)	49.15 – 3.56 49.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	62.7 (49.15-3.56) 33.5 (49.15-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.296 , 0.328 0.296 , 0.328	Depositor DCC
R_{free} test set	3544 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	99.3	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 160.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	94738	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MPT, OAS, NH2, U2X, DPR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/2639	0.42	0/3583
1	B	0.24	0/2710	0.43	0/3680
1	E	0.24	0/2612	0.41	0/3546
1	I	0.24	0/2691	0.41	0/3654
1	M	0.24	0/2675	0.42	0/3630
1	P	0.23	0/2671	0.42	0/3626
1	S	0.25	0/2677	0.43	0/3634
1	V	0.24	0/2672	0.42	0/3628
2	a	0.32	0/176	0.62	0/231
2	b	0.32	0/176	0.62	0/231
2	e	0.32	0/176	0.62	0/231
2	i	0.32	0/176	0.62	0/231
2	m	0.32	0/176	0.62	0/231
2	p	0.32	0/176	0.62	0/231
2	s	0.32	0/176	0.63	0/231
2	v	0.32	0/176	0.62	0/231
3	D	0.34	0/1646	0.65	0/2231
3	G	0.25	0/1646	0.46	0/2231
3	K	0.30	0/1646	0.57	0/2231
3	L	0.24	0/1646	0.44	0/2231
3	O	0.24	0/1646	0.44	0/2231
3	R	0.25	0/1646	0.45	0/2231
3	U	0.25	0/1646	0.46	0/2231
3	X	0.25	0/1646	0.44	0/2231
4	C	0.35	0/1713	0.71	0/2341
4	F	0.25	0/1713	0.48	0/2341
4	H	0.25	0/1713	0.46	0/2341
4	J	0.30	0/1713	0.57	0/2341
4	N	0.26	0/1713	0.59	0/2341
4	Q	0.25	0/1713	0.47	0/2341
4	T	0.27	0/1713	0.53	0/2341
4	W	0.25	0/1713	0.57	0/2341

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.26	0/49627	0.49	0/67405

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
3	K	0	1
4	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	159	LEU	Mainchain
3	K	165	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2588	2506	2508	17	0
1	B	2657	2532	2574	30	0
1	E	2561	2481	2482	13	0
1	I	2640	2532	2554	19	0
1	M	2625	2544	2543	15	0
1	P	2620	2537	2541	16	0
1	S	2626	2542	2545	31	0
1	V	2621	2539	2543	15	0
2	a	209	0	211	0	0
2	b	209	0	211	0	0
2	e	209	0	210	0	6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	i	209	0	211	0	0
2	m	209	0	211	0	0
2	p	209	0	211	0	0
2	s	209	0	211	0	2
2	v	209	0	211	0	0
3	D	1612	1584	1583	16	1
3	G	1612	1582	1583	21	2
3	K	1612	1583	1583	14	0
3	L	1612	1585	1583	3	0
3	O	1612	1586	1583	7	0
3	R	1612	1583	1583	1	0
3	U	1612	1581	1583	10	6
3	X	1612	1586	1583	4	0
4	C	1674	1571	1650	42	0
4	F	1671	1515	1647	45	0
4	H	1674	1648	1650	6	0
4	J	1671	1515	1647	39	0
4	N	1671	1651	1647	18	0
4	Q	1671	1651	1647	7	1
4	T	1674	1505	1650	37	0
4	W	1674	1647	1650	7	0
5	A	56	0	52	8	0
5	B	28	0	26	10	0
5	E	28	0	26	2	0
5	I	56	0	52	7	0
5	M	14	0	13	1	0
5	P	28	0	26	5	0
5	S	42	0	39	13	0
5	V	14	0	13	3	0
All	All	49152	45586	48076	393	9

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (393) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:100(A):LEU:HB3	4:T:100(B):PRO:HA	1.33	1.10
1:I:48:ALA:HA	1:I:49:ASN:HB2	1.28	1.09
3:G:61:ARG:HH21	3:G:79:GLN:HG3	1.14	1.08
4:J:100(A):LEU:HB3	4:J:100(B):PRO:HA	1.36	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:98:TRP:HB3	4:F:100:TYR:H	1.20	1.06
1:S:269:LYS:HB3	5:S:502:NAG:H82	1.37	1.04
4:F:100(A):LEU:HB3	4:F:100(B):PRO:HA	1.34	1.04
4:T:98:TRP:HB3	4:T:100:TYR:H	1.19	1.03
4:C:100(A):LEU:HB3	4:C:100(B):PRO:HA	1.41	0.98
3:G:61:ARG:NH2	3:G:79:GLN:CG	2.27	0.97
3:G:61:ARG:NH2	3:G:79:GLN:HG3	1.80	0.97
4:C:98:TRP:H	4:C:99:PRO:HA	1.34	0.92
4:F:98:TRP:H	4:F:99:PRO:HA	1.32	0.92
4:C:98:TRP:HB3	4:C:100:TYR:HB2	1.50	0.91
4:T:98:TRP:HB3	4:T:100:TYR:N	1.85	0.90
1:I:48:ALA:HA	1:I:49:ASN:CB	2.03	0.89
4:T:98:TRP:H	4:T:99:PRO:HA	1.38	0.89
4:T:95:ARG:HH21	4:T:100(A):LEU:HD13	1.37	0.88
3:G:61:ARG:HH21	3:G:79:GLN:CG	1.86	0.88
1:I:48:ALA:CA	1:I:49:ASN:HB2	2.05	0.86
1:B:269:LYS:HD3	5:B:502:NAG:H61	1.61	0.83
4:J:100(A):LEU:HB3	4:J:100(B):PRO:CA	2.10	0.81
1:B:269:LYS:CD	5:B:502:NAG:H61	2.12	0.79
4:J:98:TRP:HB3	4:J:100:TYR:N	1.96	0.78
4:C:98:TRP:HB3	4:C:100:TYR:N	2.00	0.77
4:J:98:TRP:H	4:J:99:PRO:HA	1.48	0.77
4:C:95:ARG:NH2	4:C:100(A):LEU:HD13	2.00	0.76
3:D:91:LEU:CD2	4:C:100(B):PRO:HB3	2.15	0.76
4:J:95:ARG:NH2	4:J:100(A):LEU:HD13	2.00	0.76
4:F:95:ARG:HH21	4:F:100(A):LEU:HD13	1.50	0.76
1:B:269:LYS:CG	5:B:502:NAG:H61	2.15	0.76
4:C:98:TRP:HB3	4:C:100:TYR:H	1.52	0.74
4:C:100(A):LEU:CB	4:C:100(B):PRO:HA	2.16	0.73
4:T:95:ARG:NH2	4:T:100(A):LEU:HD13	2.04	0.72
5:I:501:NAG:O3	5:I:501:NAG:O7	2.06	0.71
1:A:212:PRO:HG3	5:A:501:NAG:H2	1.70	0.71
4:F:98:TRP:H	4:F:99:PRO:CA	2.04	0.71
1:P:233:PHE:O	1:P:273:ARG:NH1	2.24	0.70
4:C:98:TRP:CB	4:C:100:TYR:HB2	2.20	0.70
4:F:100(A):LEU:HB3	4:F:100(B):PRO:CA	2.16	0.70
1:I:295:ASN:N	1:I:295:ASN:OD1	2.24	0.69
4:T:100(A):LEU:HB3	4:T:100(B):PRO:CA	2.16	0.69
1:S:348:GLN:NE2	5:S:502:NAG:H81	2.08	0.69
4:F:98:TRP:HB3	4:F:100:TYR:N	2.03	0.69
1:V:212:PRO:HG3	5:V:501:NAG:H2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:91:LEU:CD2	4:F:100(B):PRO:HB3	2.22	0.69
4:J:98:TRP:HB3	4:J:100:TYR:H	1.56	0.69
1:V:446:VAL:O	5:V:501:NAG:H5	1.93	0.68
3:K:36:TYR:OH	4:J:100(B):PRO:HB2	1.93	0.68
4:T:98:TRP:CB	4:T:100:TYR:H	2.02	0.68
3:D:36:TYR:OH	4:C:100(B):PRO:HB2	1.94	0.67
1:B:48:ALA:HA	1:B:490:LYS:HG3	1.77	0.67
4:F:98:TRP:CB	4:F:100:TYR:H	2.02	0.67
4:C:100(A):LEU:HB3	4:C:100(B):PRO:CA	2.23	0.67
1:B:491:ILE:HG22	1:B:492:GLU:HG3	1.75	0.67
1:B:446:VAL:O	5:B:501:NAG:H5	1.95	0.67
3:K:91:LEU:HD22	4:J:100(A):LEU:HB2	1.75	0.67
1:V:233:PHE:O	1:V:273:ARG:NH1	2.28	0.67
4:F:95:ARG:HE	4:F:100(A):LEU:HD22	1.60	0.66
4:C:98:TRP:H	4:C:99:PRO:CA	2.07	0.66
3:G:62:PHE:CE2	3:G:75:ILE:CD1	2.79	0.66
1:I:446:VAL:O	5:I:501:NAG:H3	1.96	0.66
4:N:94:ARG:NH2	4:N:101:ASP:OD1	2.29	0.66
3:D:93:GLY:O	3:D:96:ARG:NH1	2.26	0.66
5:I:501:NAG:H62	5:I:504:NAG:H81	1.77	0.66
3:K:122:ASP:OD2	4:J:214:LYS:NZ	2.29	0.66
4:F:147:PRO:O	4:F:200:HIS:NE2	2.28	0.65
1:M:232:GLU:CB	1:M:233:PHE:HA	2.27	0.65
4:Q:147:PRO:O	4:Q:200:HIS:NE2	2.30	0.65
1:B:121:GLN:NE2	1:B:426:MET:SD	2.69	0.65
3:G:62:PHE:CE2	3:G:75:ILE:HD11	2.31	0.65
3:G:91:LEU:HD22	4:F:100(B):PRO:HB3	1.78	0.65
3:G:61:ARG:NH2	3:G:79:GLN:CD	2.51	0.64
4:J:33:TYR:CE1	4:J:52:LYS:HB2	2.33	0.64
4:C:98:TRP:HB3	4:C:100:TYR:CB	2.26	0.64
1:P:269:LYS:HD3	5:P:502:NAG:H61	1.80	0.64
1:S:298:ARG:NH2	1:S:441:GLY:O	2.31	0.64
4:H:30:OAS:HC22	4:H:31:GLY:H	1.62	0.63
4:T:100(A):LEU:CB	4:T:100(B):PRO:HA	2.20	0.63
1:E:232:GLU:CB	1:E:233:PHE:HA	2.28	0.62
1:S:270:VAL:O	1:S:348:GLN:NE2	2.31	0.62
4:F:100(A):LEU:CB	4:F:100(B):PRO:HA	2.22	0.62
4:J:95:ARG:HH21	4:J:100(A):LEU:HD13	1.62	0.62
1:I:261:LEU:HD13	5:I:501:NAG:H83	1.81	0.62
1:A:269:LYS:HE2	5:A:502:NAG:H4	1.81	0.62
4:F:117:LYS:HB2	3:U:126:LYS:HZ2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:232:GLU:CB	1:P:233:PHE:HA	2.30	0.62
1:V:232:GLU:CB	1:V:233:PHE:HA	2.29	0.61
3:G:61:ARG:NH2	3:G:79:GLN:CB	2.63	0.61
4:J:98:TRP:HB3	4:J:100:TYR:HB2	1.81	0.61
4:T:98:TRP:N	4:T:99:PRO:HA	2.12	0.61
3:O:37:GLN:O	3:O:45:LYS:N	2.33	0.61
1:M:298:ARG:NH2	1:M:441:GLY:O	2.34	0.60
3:U:91:LEU:HD22	4:T:100(B):PRO:HB3	1.81	0.60
4:J:100(A):LEU:CB	4:J:100(B):PRO:CA	2.80	0.60
4:F:33:TYR:CE2	4:F:52:LYS:HD3	2.36	0.60
1:S:232:GLU:CB	1:S:233:PHE:HA	2.32	0.60
1:B:287:GLN:NE2	1:B:481:SER:O	2.35	0.60
1:M:66:HIS:ND1	1:M:211:GLU:O	2.35	0.60
1:I:66:HIS:ND1	1:I:211:GLU:O	2.35	0.59
1:I:232:GLU:CB	1:I:233:PHE:HA	2.31	0.59
1:P:344:GLN:OE1	5:P:502:NAG:H62	2.01	0.59
4:J:52:LYS:HG3	4:J:54:ASN:H	1.68	0.59
4:J:57:PRO:HB2	4:J:59:TYR:CZ	2.38	0.59
1:S:212:PRO:HG3	5:S:501:NAG:H2	1.84	0.59
3:G:61:ARG:HH22	3:G:79:GLN:HB2	1.67	0.59
1:M:368:ASP:OD2	1:M:425:ASN:ND2	2.36	0.59
1:A:344:GLN:OE1	5:A:502:NAG:H62	2.02	0.58
1:E:353:TRP:O	1:E:357:ASN:ND2	2.36	0.57
4:F:95:ARG:NH2	4:F:100(A):LEU:HD13	2.19	0.57
1:I:327:ARG:NH2	1:I:422:GLN:OE1	2.37	0.57
1:B:232:GLU:CB	1:B:233:PHE:HA	2.34	0.57
1:S:348:GLN:HE21	5:S:502:NAG:H81	1.70	0.57
4:T:33:TYR:CE1	4:T:52:LYS:HB2	2.38	0.57
1:V:212:PRO:CG	5:V:501:NAG:H2	2.34	0.57
1:P:269:LYS:HE2	5:P:502:NAG:H4	1.87	0.57
3:K:93:GLY:O	3:K:96:ARG:NH1	2.34	0.57
1:V:66:HIS:ND1	1:V:211:GLU:O	2.38	0.57
1:S:66:HIS:ND1	1:S:211:GLU:O	2.37	0.57
3:D:91:LEU:HD22	4:C:100(B):PRO:HB3	1.86	0.56
3:U:91:LEU:HD21	4:T:100(B):PRO:HG3	1.86	0.56
3:G:61:ARG:NH2	3:G:79:GLN:HB2	2.21	0.56
1:S:290:GLU:OE2	5:S:502:NAG:O6	2.20	0.56
1:A:212:PRO:CG	5:A:501:NAG:H2	2.35	0.56
4:J:55:GLY:O	4:J:57:PRO:HD3	2.06	0.56
1:P:446:VAL:O	5:P:501:NAG:H5	2.05	0.56
1:E:446:VAL:O	5:E:501:NAG:H5	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:126:LYS:HD2	4:T:115:SER:HB2	1.88	0.55
1:E:66:HIS:ND1	1:E:211:GLU:O	2.39	0.55
4:J:197:ASN:OD1	4:J:197:ASN:N	2.38	0.55
4:T:55:GLY:O	4:T:57:PRO:HD3	2.07	0.55
4:T:98:TRP:HB3	4:T:100:TYR:HB2	1.89	0.55
4:W:197:ASN:N	4:W:197:ASN:OD1	2.41	0.54
1:P:447:SER:OG	5:P:501:NAG:N2	2.41	0.54
4:F:95:ARG:NE	4:F:100(A):LEU:HD22	2.21	0.54
4:Q:197:ASN:OD1	4:Q:197:ASN:N	2.39	0.54
1:S:446:VAL:O	5:S:501:NAG:H5	2.08	0.53
4:T:52:LYS:HG3	4:T:53:HIS:N	2.22	0.53
1:E:77:THR:O	4:F:33:TYR:OH	2.24	0.53
1:M:232:GLU:HB2	1:M:233:PHE:HA	1.90	0.53
4:T:100(A):LEU:CB	4:T:100(B):PRO:CA	2.85	0.53
1:A:66:HIS:ND1	1:A:211:GLU:O	2.41	0.53
4:F:95:ARG:HH21	4:F:100(A):LEU:CD1	2.20	0.53
4:J:98:TRP:N	4:J:99:PRO:HA	2.22	0.53
4:F:57:PRO:HB2	4:F:59:TYR:CE2	2.43	0.53
5:B:502:NAG:O3	5:B:502:NAG:O7	2.23	0.53
4:C:33:TYR:HB2	4:C:95:ARG:HB2	1.91	0.53
1:A:99:ASN:OD1	1:A:103:GLN:NE2	2.42	0.53
4:F:52:LYS:HG3	4:F:53:HIS:N	2.24	0.53
4:F:98:TRP:HB3	4:F:100:TYR:HB2	1.91	0.53
1:I:232:GLU:HB2	1:I:233:PHE:HA	1.91	0.53
4:C:121:VAL:HG12	4:C:209:LYS:HD2	1.92	0.52
3:U:91:LEU:CD2	4:T:100(B):PRO:HG3	2.39	0.52
3:X:164:THR:HG21	4:W:164:HIS:HB3	1.92	0.52
1:E:232:GLU:HB2	1:E:233:PHE:HA	1.90	0.52
4:J:129:LYS:H	4:J:129:LYS:HD3	1.74	0.52
3:G:62:PHE:HE2	3:G:75:ILE:HD11	1.73	0.52
1:A:335:GLY:O	1:A:339:ASN:ND2	2.42	0.52
1:I:211:GLU:OE2	5:I:501:NAG:H4	2.10	0.52
1:M:55:ALA:N	1:M:216:HIS:O	2.43	0.52
3:G:61:ARG:NH2	3:G:82:ASP:OD2	2.43	0.52
4:T:33:TYR:CE1	4:T:52:LYS:HD3	2.45	0.52
4:F:100:TYR:C	4:F:100(A):LEU:HG	2.31	0.51
1:V:335:GLY:O	1:V:339:ASN:ND2	2.42	0.51
4:H:55:GLY:O	4:H:56:SER:OG	2.25	0.51
1:P:232:GLU:HB2	1:P:233:PHE:HA	1.93	0.51
4:C:95:ARG:HD3	4:C:100(C):PHE:CE1	2.45	0.51
4:W:12:LEU:HD11	4:W:18:LEU:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:91:LEU:HD21	4:C:100(B):PRO:HB3	1.90	0.51
4:C:95:ARG:HB3	4:C:100(A):LEU:CD2	2.41	0.51
1:M:232:GLU:HB3	1:M:233:PHE:HA	1.93	0.50
4:F:57:PRO:HB2	4:F:59:TYR:CZ	2.47	0.50
4:N:100(A):LEU:N	4:N:100(B):PRO:HD2	2.26	0.50
1:V:232:GLU:HB2	1:V:233:PHE:HA	1.93	0.50
1:B:212:PRO:HG3	5:B:501:NAG:H2	1.94	0.50
4:J:52:LYS:HG3	4:J:53:HIS:N	2.26	0.50
4:Q:100(A):LEU:N	4:Q:100(B):PRO:CD	2.75	0.50
4:F:95:ARG:HD3	4:F:100(C):PHE:CD1	2.47	0.50
5:I:501:NAG:H62	5:I:504:NAG:C8	2.41	0.50
4:C:25:TYR:OH	1:S:86:MET:SD	2.52	0.50
4:T:98:TRP:H	4:T:99:PRO:CA	2.16	0.50
4:F:129:LYS:HD3	4:F:129:LYS:H	1.77	0.49
4:J:98:TRP:CB	4:J:100:TYR:HB2	2.42	0.49
3:O:61:ARG:NH2	3:O:81:GLU:OE2	2.43	0.49
1:E:388:SER:OG	5:E:502:NAG:H62	2.13	0.49
1:S:269:LYS:HA	1:S:289:ASN:HD22	1.76	0.49
1:A:269:LYS:HD3	5:A:502:NAG:H61	1.95	0.49
4:C:150:VAL:HG12	4:C:200:HIS:HB2	1.93	0.49
1:A:87:GLU:OE1	1:A:87:GLU:N	2.45	0.49
3:X:186:TYR:O	3:X:192:TYR:OH	2.30	0.49
3:X:37:GLN:O	3:X:45:LYS:N	2.46	0.49
4:H:100(A):LEU:N	4:H:100(B):PRO:CD	2.76	0.48
4:F:206:LYS:HB2	4:T:208:ASP:HB2	1.95	0.48
4:C:144:ASP:OD1	4:C:171:GLN:NE2	2.47	0.48
4:F:95:ARG:HH21	4:F:100(A):LEU:HD22	1.78	0.48
1:B:233:PHE:O	1:B:273:ARG:NH1	2.46	0.48
1:S:99:ASN:OD1	1:S:103:GLN:NE2	2.44	0.48
4:F:50:GLU:OE1	4:F:95:ARG:NH1	2.47	0.48
1:I:350:ARG:O	1:I:352:TYR:N	2.46	0.48
4:T:33:TYR:CZ	4:T:52:LYS:HD3	2.49	0.48
4:C:165:THR:HG22	4:C:165:THR:O	2.13	0.48
4:H:129:LYS:HD3	4:H:129:LYS:H	1.79	0.48
4:F:115:SER:HB2	3:U:126:LYS:HD2	1.94	0.48
1:B:46:LYS:HD2	1:B:491:ILE:HD13	1.96	0.47
4:J:33:TYR:CE1	4:J:52:LYS:HD3	2.48	0.47
1:P:66:HIS:ND1	1:P:211:GLU:O	2.47	0.47
1:S:269:LYS:HG2	5:S:502:NAG:HN2	1.79	0.47
1:S:344:GLN:OE1	5:S:502:NAG:O3	2.28	0.47
4:F:100(A):LEU:CB	4:F:100(B):PRO:CA	2.89	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:34:TRP:CH2	4:N:94:ARG:HG3	2.49	0.47
3:O:164:THR:HG21	4:N:164:HIS:HB3	1.96	0.47
1:B:232:GLU:HB2	1:B:233:PHE:HA	1.96	0.47
4:J:50:GLU:OE1	4:J:95:ARG:NH1	2.48	0.47
1:V:232:GLU:HB3	1:V:233:PHE:HA	1.96	0.47
4:W:129:LYS:H	4:W:129:LYS:HD3	1.78	0.47
3:D:108:ARG:NH1	3:D:111:ALA:HB2	2.30	0.47
1:M:461:ASN:O	1:M:463:ASN:N	2.47	0.47
1:S:348:GLN:NE2	5:S:502:NAG:C8	2.76	0.47
1:B:46:LYS:HD2	1:B:491:ILE:CD1	2.44	0.47
1:M:232:GLU:CB	1:M:233:PHE:CA	2.92	0.47
4:N:29:LEU:HD23	4:N:34:TRP:CZ2	2.50	0.47
1:S:344:GLN:HB3	5:S:502:NAG:O7	2.15	0.47
1:S:232:GLU:CB	1:S:233:PHE:CA	2.93	0.46
1:P:232:GLU:HB3	1:P:233:PHE:HA	1.98	0.46
1:S:232:GLU:HB3	1:S:233:PHE:HA	1.97	0.46
4:F:98:TRP:N	4:F:99:PRO:CA	2.75	0.46
4:C:100(A):LEU:CB	4:C:100(B):PRO:CA	2.88	0.46
1:A:350:ARG:O	1:A:352:TYR:N	2.45	0.46
3:K:37:GLN:O	3:K:45:LYS:N	2.47	0.46
1:A:278:THR:HG22	5:A:504:NAG:H62	1.98	0.46
4:N:34:TRP:CZ3	4:N:94:ARG:HB2	2.50	0.46
1:M:218:CYS:HB2	4:N:98:TRP:CZ2	2.51	0.46
3:U:36:TYR:OH	4:T:100(B):PRO:HG2	2.16	0.46
1:V:232:GLU:CB	1:V:233:PHE:CA	2.94	0.46
4:J:38:ARG:HB3	4:J:48:ILE:HD11	1.97	0.46
1:M:446:VAL:O	5:M:501:NAG:H5	2.16	0.46
3:K:34:ALA:CB	4:J:100(B):PRO:HG3	2.46	0.46
1:S:232:GLU:HB2	1:S:233:PHE:HA	1.97	0.46
3:U:93:GLY:O	3:U:96:ARG:NH1	2.34	0.46
4:C:143:LYS:HG3	4:C:177:SER:HB2	1.97	0.46
1:S:65:VAL:HB	1:S:115:SER:HB3	1.97	0.46
1:E:232:GLU:HB3	1:E:233:PHE:HA	1.97	0.45
3:O:10:PHE:CZ	3:O:105:GLU:HG2	2.51	0.45
1:B:269:LYS:CB	5:B:502:NAG:H61	2.46	0.45
4:J:98:TRP:H	4:J:99:PRO:CA	2.24	0.45
1:S:348:GLN:HE21	5:S:502:NAG:C8	2.29	0.45
3:K:6:GLN:HE22	3:K:87:TYR:HA	1.81	0.45
3:L:61:ARG:NH2	3:L:81:GLU:OE2	2.49	0.45
1:A:94:ASN:OD1	1:A:97:LYS:N	2.50	0.45
1:B:269:LYS:HG2	1:B:348:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:60:HIS:CG	4:T:61:PRO:HD2	2.52	0.45
1:B:270:VAL:HG22	1:B:288:LEU:HA	1.98	0.45
1:P:112:TRP:CE3	1:P:427:TRP:CZ2	3.05	0.45
4:Q:152:VAL:HG11	4:Q:180:SER:CB	2.47	0.45
4:N:152:VAL:HG11	4:N:180:SER:CB	2.47	0.45
1:V:257:THR:O	1:V:259:LEU:N	2.49	0.44
4:C:98:TRP:HB3	4:C:100:TYR:CA	2.47	0.44
1:E:232:GLU:CB	1:E:233:PHE:CA	2.94	0.44
3:O:166:GLN:HG3	3:O:173:TYR:CZ	2.52	0.44
1:B:270:VAL:HB	1:B:348:GLN:HE22	1.82	0.44
3:K:36:TYR:HH	4:J:100(B):PRO:HB2	1.83	0.44
4:Q:129:LYS:HD3	4:Q:129:LYS:H	1.82	0.44
4:F:175:LEU:HD21	3:U:126:LYS:NZ	2.32	0.44
4:C:200:HIS:CE1	4:C:202:PRO:HB2	2.53	0.44
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.53	0.44
1:B:327:ARG:NH2	1:B:422:GLN:OE1	2.49	0.44
4:C:100(B):PRO:HB2	4:C:100(C):PHE:H	1.62	0.44
4:N:188:SER:O	4:N:192:GLN:N	2.50	0.44
4:W:100(A):LEU:N	4:W:100(B):PRO:HD2	2.31	0.44
1:A:77:THR:HB	1:A:78:ASP:CB	2.47	0.44
1:B:48:ALA:HB1	1:B:488:VAL:HG12	2.00	0.44
4:C:116:THR:CG2	4:C:203:SER:HB3	2.48	0.44
4:F:95:ARG:HD3	4:F:100(C):PHE:CE1	2.53	0.44
3:G:61:ARG:CZ	3:G:79:GLN:NE2	2.81	0.44
1:P:232:GLU:CB	1:P:233:PHE:CA	2.95	0.44
3:K:118:PHE:HB3	4:J:124:LEU:HD22	1.99	0.44
4:T:98:TRP:N	4:T:99:PRO:CA	2.79	0.44
4:C:12:LEU:HD11	4:C:18:LEU:HA	2.00	0.44
1:E:76:PRO:O	1:E:77:THR:OG1	2.24	0.44
4:F:33:TYR:HB2	4:F:95:ARG:HB2	2.00	0.44
1:I:295:ASN:HD22	1:I:444:ARG:NH2	2.15	0.44
1:S:269:LYS:HD3	5:S:502:NAG:C8	2.48	0.44
3:D:58:VAL:HA	3:D:59:PRO:HD3	1.90	0.43
3:G:126:LYS:HZ1	4:T:175:LEU:HD21	1.83	0.43
1:S:269:LYS:HD3	5:S:502:NAG:H83	1.99	0.43
4:W:100(A):LEU:N	4:W:100(B):PRO:CD	2.81	0.43
3:O:46:LEU:HD22	4:N:100(B):PRO:HB2	2.01	0.43
4:C:95:ARG:HB3	4:C:100(A):LEU:HD22	2.01	0.43
1:B:61:TYR:HD2	4:C:61:PRO:HA	1.83	0.43
4:H:100(A):LEU:N	4:H:100(B):PRO:HD2	2.34	0.43
1:I:105:HIS:CE1	1:I:427:TRP:CZ2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:68:THR:HB	4:J:81:ASN:HB2	2.00	0.43
4:T:129:LYS:HD3	4:T:129:LYS:H	1.82	0.43
3:D:209:PHE:HB3	4:C:129:LYS:NZ	2.33	0.43
4:F:12:LEU:HD11	4:F:18:LEU:HA	2.00	0.43
4:J:98:TRP:HB3	4:J:100:TYR:CB	2.49	0.43
1:A:71:THR:HG22	3:L:93:GLY:HA2	2.01	0.43
1:M:76:PRO:O	1:M:77:THR:OG1	2.22	0.43
4:N:129:LYS:H	4:N:129:LYS:HD3	1.82	0.43
3:U:33:LEU:HD22	3:U:71:PHE:CD1	2.53	0.43
4:F:95:ARG:NH2	4:F:100(A):LEU:HD22	2.33	0.43
4:J:97:ASN:O	4:J:98:TRP:HB2	2.18	0.43
1:B:290:GLU:OE2	5:B:502:NAG:H82	2.19	0.43
1:A:386:ASN:HD22	5:A:503:NAG:H83	1.84	0.43
1:B:61:TYR:CG	4:C:64:LYS:HD3	2.53	0.43
4:N:90:TYR:CD1	4:N:90:TYR:N	2.86	0.43
1:V:77:THR:HB	1:V:78:ASP:HA	2.01	0.43
1:V:77:THR:HB	1:V:78:ASP:HB3	2.01	0.43
1:B:48:ALA:HB2	1:B:489:VAL:HA	2.01	0.42
5:I:504:NAG:O7	5:I:504:NAG:O3	2.29	0.42
1:P:77:THR:HB	1:P:78:ASP:HB3	1.99	0.42
4:T:119:PRO:HB3	4:T:145:TYR:HB3	2.01	0.42
4:T:201:LYS:N	4:T:202:PRO:CD	2.82	0.42
4:F:203:SER:O	4:T:209:LYS:NZ	2.51	0.42
4:C:147:PRO:O	4:C:200:HIS:NE2	2.48	0.42
4:F:33:TYR:CZ	4:F:52:LYS:HD3	2.54	0.42
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.54	0.42
3:K:44:PRO:HG3	4:J:45:LEU:HD11	2.00	0.42
1:B:269:LYS:HG3	5:B:502:NAG:H61	1.96	0.42
3:D:185:ASP:O	3:D:188:LYS:HG2	2.19	0.42
3:D:191:VAL:HG22	3:D:210:ASN:OD1	2.18	0.42
4:F:51:ILE:HG13	4:F:52:LYS:N	2.33	0.42
4:J:94:ARG:O	4:J:100(C):PHE:HA	2.20	0.42
4:N:95:ARG:HA	4:N:100(C):PHE:HB3	2.01	0.42
4:N:98:TRP:CD1	4:N:99:PRO:HA	2.54	0.42
1:B:232:GLU:CB	1:B:233:PHE:CA	2.96	0.42
4:C:197:ASN:N	4:C:197:ASN:OD1	2.53	0.42
4:C:75:LYS:HG2	1:S:85:LYS:HD2	2.02	0.42
1:M:257:THR:O	1:M:259:LEU:N	2.51	0.42
3:O:43:ALA:HB1	4:N:103:TRP:HB2	2.02	0.42
4:Q:12:LEU:HD11	4:Q:18:LEU:HA	2.01	0.42
4:C:98:TRP:N	4:C:99:PRO:CA	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:178:LEU:HD23	4:T:178:LEU:C	2.40	0.42
4:T:57:PRO:HB2	4:T:59:TYR:CE2	2.55	0.42
1:A:278:THR:CG2	5:A:504:NAG:H62	2.50	0.42
3:G:91:LEU:HD21	4:F:100(B):PRO:HG3	2.02	0.42
1:P:112:TRP:CE3	1:P:427:TRP:CH2	3.07	0.42
1:S:61:TYR:CG	4:T:64:LYS:HD3	2.54	0.42
3:D:89:GLN:NE2	4:C:100(C):PHE:HE2	2.18	0.42
1:I:77:THR:HB	1:I:78:ASP:HB3	2.02	0.42
1:E:373:THR:O	1:E:374:HIS:CB	2.68	0.42
3:K:124:GLN:HG3	4:J:122:PHE:CE2	2.55	0.42
4:T:12:LEU:HD11	4:T:18:LEU:HA	2.02	0.42
4:N:28:SER:OG	4:N:29:LEU:N	2.41	0.41
4:Q:38:ARG:NH2	4:Q:46:GLU:OE1	2.52	0.41
1:B:212:PRO:CG	5:B:501:NAG:H2	2.50	0.41
1:I:48:ALA:CB	1:I:49:ASN:HB2	2.50	0.41
3:K:13:ALA:HB3	3:K:104:LEU:HD11	2.02	0.41
1:I:298:ARG:NH2	1:I:441:GLY:O	2.52	0.41
4:J:127:SER:HB2	4:J:129:LYS:HD3	2.02	0.41
4:J:132:SER:N	4:J:135:THR:O	2.53	0.41
1:S:55:ALA:N	1:S:216:HIS:O	2.53	0.41
3:X:116:PHE:CE2	4:W:132:SER:HB2	2.56	0.41
4:J:51:ILE:HG13	4:J:52:LYS:N	2.35	0.41
4:F:100(B):PRO:HB2	4:F:100(C):PHE:H	1.53	0.41
1:B:45:TRP:O	1:B:47:ASP:N	2.51	0.41
4:C:201:LYS:N	4:C:202:PRO:CD	2.84	0.41
1:I:232:GLU:CB	1:I:233:PHE:CA	2.96	0.41
1:M:201:LEU:HD23	1:M:202:THR:N	2.35	0.41
4:N:103:TRP:N	4:N:103:TRP:CD1	2.88	0.41
4:T:52:LYS:HG3	4:T:54:ASN:H	1.85	0.41
1:V:66:HIS:CE1	1:V:212:PRO:HA	2.55	0.41
4:J:119:PRO:HB3	4:J:145:TYR:HB3	2.03	0.41
1:P:350:ARG:O	1:P:352:TYR:N	2.46	0.41
1:A:77:THR:HB	1:A:78:ASP:CA	2.51	0.41
1:E:374:HIS:CD2	1:E:375:SER:N	2.89	0.41
3:G:209:PHE:HB3	4:F:129:LYS:NZ	2.35	0.41
3:D:149:LYS:N	3:D:193:ALA:O	2.43	0.41
3:G:62:PHE:CZ	3:G:75:ILE:HD13	2.56	0.41
3:L:49:TYR:HB3	4:H:100(B):PRO:HG3	2.03	0.41
1:M:96:TRP:CD2	1:M:275:GLU:HG3	2.56	0.41
1:S:83:GLU:OE2	1:S:227:LYS:NZ	2.52	0.41
4:F:150:VAL:HG12	4:F:200:HIS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:108:ARG:HH21	3:K:170:ASP:HB2	1.86	0.40
3:K:185:ASP:O	3:K:188:LYS:HG2	2.21	0.40
1:S:76:PRO:O	1:S:77:THR:OG1	2.32	0.40
4:C:127:SER:OG	4:C:129:LYS:CE	2.69	0.40
3:D:142:ARG:O	3:D:142:ARG:HG2	2.20	0.40
3:D:158:ASN:O	3:D:179:LEU:HD12	2.21	0.40
1:P:55:ALA:N	1:P:216:HIS:O	2.54	0.40
1:V:55:ALA:N	1:V:216:HIS:O	2.53	0.40
1:B:65:VAL:HB	1:B:115:SER:HB3	2.04	0.40
4:N:105:GLN:N	4:N:105:GLN:OE1	2.44	0.40
3:R:33:LEU:HD22	3:R:71:PHE:CG	2.57	0.40
4:C:159:LEU:HD21	4:C:182:VAL:HG21	2.03	0.40
1:E:325:ASP:OD1	1:E:326:ILE:N	2.54	0.40
4:F:175:LEU:HD21	3:U:126:LYS:HZ1	1.85	0.40
1:I:48:ALA:HB3	1:I:488:VAL:HG12	2.03	0.40
4:J:33:TYR:CZ	4:J:52:LYS:HD3	2.57	0.40
1:B:232:GLU:HB3	1:B:233:PHE:HA	2.04	0.40
3:D:33:LEU:HG	3:D:34:ALA:N	2.37	0.40
1:S:61:TYR:HD2	4:T:61:PRO:HA	1.87	0.40
1:S:77:THR:HB	1:S:78:ASP:CB	2.51	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:e:3:LEU:CD1	3:U:24:ARG:CZ[1_545]	1.75	0.45
2:e:3:LEU:CD1	3:U:24:ARG:NH1[1_545]	1.75	0.45
2:e:7:GLN:NE2	3:U:24:ARG:NH2[1_545]	1.84	0.36
2:e:7:GLN:CD	3:U:24:ARG:NH2[1_545]	2.01	0.19
3:G:24:ARG:NH2	2:s:7:GLN:NE2[1_545]	2.05	0.15
2:e:7:GLN:NE2	3:U:24:ARG:HH21[1_545]	1.55	0.05
2:e:3:LEU:CD2	3:U:24:ARG:NE[1_545]	2.16	0.04
3:G:24:ARG:HH22	2:s:7:GLN:NE2[1_545]	1.57	0.03
3:D:126:LYS:HZ2	4:Q:115:SER:O[1_565]	1.59	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/352 (93%)	298 (91%)	26 (8%)	3 (1%)	20	63
1	B	336/352 (96%)	301 (90%)	29 (9%)	6 (2%)	10	50
1	E	323/352 (92%)	290 (90%)	26 (8%)	7 (2%)	8	46
1	I	335/352 (95%)	285 (85%)	42 (12%)	8 (2%)	7	44
1	M	333/352 (95%)	298 (90%)	28 (8%)	7 (2%)	8	47
1	P	332/352 (94%)	295 (89%)	30 (9%)	7 (2%)	8	47
1	S	333/352 (95%)	293 (88%)	34 (10%)	6 (2%)	10	50
1	V	332/352 (94%)	299 (90%)	29 (9%)	4 (1%)	15	58
2	a	24/28 (86%)	24 (100%)	0	0	100	100
2	b	24/28 (86%)	24 (100%)	0	0	100	100
2	e	24/28 (86%)	24 (100%)	0	0	100	100
2	i	24/28 (86%)	24 (100%)	0	0	100	100
2	m	24/28 (86%)	24 (100%)	0	0	100	100
2	p	24/28 (86%)	24 (100%)	0	0	100	100
2	s	24/28 (86%)	24 (100%)	0	0	100	100
2	v	24/28 (86%)	24 (100%)	0	0	100	100
3	D	208/210 (99%)	194 (93%)	13 (6%)	1 (0%)	32	73
3	G	208/210 (99%)	197 (95%)	11 (5%)	0	100	100
3	K	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	L	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	O	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
3	R	208/210 (99%)	197 (95%)	11 (5%)	0	100	100
3	U	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
3	X	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
4	C	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	13	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	10	50
4	H	217/220 (99%)	204 (94%)	13 (6%)	0	100	100
4	J	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	10	50
4	N	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	13	55
4	Q	217/220 (99%)	203 (94%)	13 (6%)	1 (0%)	32	73
4	T	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	13	55
4	W	217/220 (99%)	198 (91%)	18 (8%)	1 (0%)	32	73
All	All	6243/6480 (96%)	5748 (92%)	427 (7%)	68 (1%)	17	60

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	B	81	PRO
1	I	81	PRO
4	C	98	TRP
4	C	100(A)	LEU
1	E	81	PRO
1	E	232	GLU
4	F	98	TRP
4	F	100(B)	PRO
4	J	98	TRP
4	J	100(A)	LEU
4	J	100(B)	PRO
1	M	81	PRO
1	M	232	GLU
4	N	53	HIS
4	N	102	PRO
1	P	81	PRO
1	P	232	GLU
1	S	72	HIS
1	S	81	PRO
4	T	98	TRP
4	T	100(B)	PRO
1	V	81	PRO
1	V	232	GLU
1	B	467	THR
1	I	49	ASN
4	C	100(B)	PRO
1	E	72	HIS

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Mol	Chain	Res	Type
1	M	62	ASP
1	P	62	ASP
1	P	72	HIS
1	P	467	THR
1	S	232	GLU
1	S	409	ILE
1	S	467	THR
4	T	100(A)	LEU
1	V	467	THR
4	W	28	SER
1	A	467	THR
1	B	232	GLU
1	I	72	HIS
1	I	258	GLN
1	E	62	ASP
1	E	374	HIS
1	E	467	THR
1	M	462	SER
1	M	467	THR
4	N	130	SER
1	A	350	ARG
1	B	491	ILE
1	I	232	GLU
1	I	406	THR
1	I	409	ILE
1	E	243	SER
4	F	100	TYR
4	F	100(A)	LEU
1	M	406	THR
1	P	350	ARG
1	S	406	THR
1	I	467	THR
4	J	130	SER
1	M	73	ALA
1	V	73	ALA
1	B	76	PRO
1	B	409	ILE
3	D	110	VAL
1	P	409	ILE
4	Q	100(A)	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/306 (96%)	287 (98%)	6 (2%)	60	85
1	B	299/306 (98%)	297 (99%)	2 (1%)	87	95
1	E	290/306 (95%)	288 (99%)	2 (1%)	87	95
1	I	298/306 (97%)	291 (98%)	7 (2%)	56	83
1	M	296/306 (97%)	293 (99%)	3 (1%)	80	91
1	P	295/306 (96%)	289 (98%)	6 (2%)	60	85
1	S	296/306 (97%)	290 (98%)	6 (2%)	60	85
1	V	296/306 (97%)	286 (97%)	10 (3%)	42	77
2	a	20/20 (100%)	19 (95%)	1 (5%)	28	66
2	b	20/20 (100%)	20 (100%)	0	100	100
2	e	20/20 (100%)	20 (100%)	0	100	100
2	i	20/20 (100%)	20 (100%)	0	100	100
2	m	20/20 (100%)	20 (100%)	0	100	100
2	p	20/20 (100%)	20 (100%)	0	100	100
2	s	20/20 (100%)	20 (100%)	0	100	100
2	v	20/20 (100%)	20 (100%)	0	100	100
3	D	183/183 (100%)	176 (96%)	7 (4%)	38	73
3	G	183/183 (100%)	179 (98%)	4 (2%)	57	84
3	K	183/183 (100%)	182 (100%)	1 (0%)	91	97
3	L	183/183 (100%)	181 (99%)	2 (1%)	78	91
3	O	183/183 (100%)	180 (98%)	3 (2%)	68	88
3	R	183/183 (100%)	180 (98%)	3 (2%)	68	88
3	U	183/183 (100%)	178 (97%)	5 (3%)	50	80
3	X	183/183 (100%)	180 (98%)	3 (2%)	68	88
4	C	190/190 (100%)	180 (95%)	10 (5%)	26	65
4	F	190/190 (100%)	184 (97%)	6 (3%)	44	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	190/190 (100%)	186 (98%)	4 (2%)	59	85
4	J	190/190 (100%)	185 (97%)	5 (3%)	51	81
4	N	190/190 (100%)	179 (94%)	11 (6%)	23	62
4	Q	190/190 (100%)	187 (98%)	3 (2%)	68	88
4	T	190/190 (100%)	184 (97%)	6 (3%)	44	77
4	W	190/190 (100%)	183 (96%)	7 (4%)	39	74
All	All	5507/5592 (98%)	5384 (98%)	123 (2%)	57	84

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	GLU
1	A	244	THR
1	A	343	HIS
1	A	418	CYS
1	A	429	ARG
1	A	440	GLN
1	B	49	ASN
1	B	387	THR
2	a	11	LYS
3	L	72	THR
3	L	108	ARG
1	I	47	ASP
1	I	53	PHE
1	I	80	SER
1	I	107	ASP
1	I	201	LEU
1	I	295	ASN
1	I	343	HIS
4	H	95	ARG
4	H	129	LYS
4	H	178	LEU
4	H	197	ASN
3	D	24	ARG
3	D	37	GLN
3	D	69	THR
3	D	72	THR
3	D	81	GLU
3	D	108	ARG
3	D	134	CYS

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Mol	Chain	Res	Type
4	C	38	ARG
4	C	63	LEU
4	C	100	TYR
4	C	129	LYS
4	C	177	SER
4	C	178	LEU
4	C	179	SER
4	C	197	ASN
4	C	208	ASP
4	C	209	LYS
1	E	53	PHE
1	E	387	THR
3	G	61	ARG
3	G	72	THR
3	G	105	GLU
3	G	108	ARG
4	F	129	LYS
4	F	140	CYS
4	F	160	THR
4	F	178	LEU
4	F	197	ASN
4	F	208	ASP
3	K	108	ARG
4	J	101	ASP
4	J	129	LYS
4	J	178	LEU
4	J	186	SER
4	J	197	ASN
1	M	53	PHE
1	M	368	ASP
1	M	387	THR
3	O	72	THR
3	O	105	GLU
3	O	108	ARG
4	N	13	LYS
4	N	50	GLU
4	N	51	ILE
4	N	52	LYS
4	N	92	CYS
4	N	98	TRP
4	N	100	TYR
4	N	103	TRP

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Mol	Chain	Res	Type
4	N	129	LYS
4	N	178	LEU
4	N	194	TYR
1	P	53	PHE
1	P	80	SER
1	P	201	LEU
1	P	239	CYS
1	P	276	ASN
1	P	343	HIS
3	R	72	THR
3	R	105	GLU
3	R	108	ARG
4	Q	129	LYS
4	Q	178	LEU
4	Q	197	ASN
1	S	80	SER
1	S	201	LEU
1	S	276	ASN
1	S	289	ASN
1	S	343	HIS
1	S	387	THR
3	U	7	SER
3	U	72	THR
3	U	81	GLU
3	U	89	GLN
3	U	108	ARG
4	T	129	LYS
4	T	177	SER
4	T	178	LEU
4	T	179	SER
4	T	197	ASN
4	T	209	LYS
1	V	53	PHE
1	V	64	GLU
1	V	71	THR
1	V	74	CYS
1	V	201	LEU
1	V	239	CYS
1	V	343	HIS
1	V	387	THR
1	V	464	GLU
1	V	487	LYS

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Mol	Chain	Res	Type
3	X	72	THR
3	X	105	GLU
3	X	108	ARG
4	W	13	LYS
4	W	95	ARG
4	W	129	LYS
4	W	178	LEU
4	W	194	TYR
4	W	196	CYS
4	W	197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	105	HIS
2	b	7	GLN
1	E	357	ASN
2	m	7	GLN
1	P	374	HIS
3	U	89	GLN
2	v	7	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues 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
4	OAS	C	30	4	8,8,9	1.03	1 (12%)	6,9,11	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OAS	F	30	4	5,5,9	1.14	0	1,5,11	0.26	0
4	OAS	H	30	4	8,8,9	1.01	1 (12%)	6,9,11	0.78	0
4	OAS	J	30	4	5,5,9	1.14	1 (20%)	1,5,11	0.51	0
4	OAS	N	30	4	5,5,9	1.11	0	1,5,11	0.49	0
4	OAS	Q	30	4	5,5,9	1.18	1 (20%)	1,5,11	0.22	0
4	OAS	T	30	4	8,8,9	0.92	0	6,9,11	0.68	0
4	OAS	W	30	4	8,8,9	0.93	0	6,9,11	0.61	0
2	DPR	a	21	2	6,7,8	0.81	0	7,8,10	1.22	1 (14%)
2	U2X	a	23	2	20,20,21	2.22	4 (20%)	24,25,27	1.90	7 (29%)
2	DPR	b	21	2	6,7,8	0.81	0	7,8,10	1.22	1 (14%)
2	U2X	b	23	2	20,20,21	2.23	4 (20%)	24,25,27	1.90	7 (29%)
2	DPR	e	21	2	6,7,8	0.82	0	7,8,10	1.22	1 (14%)
2	U2X	e	23	2	20,20,21	2.22	5 (25%)	24,25,27	1.90	7 (29%)
2	DPR	i	21	2	6,7,8	0.82	0	7,8,10	1.22	1 (14%)
2	U2X	i	23	2	20,20,21	2.23	4 (20%)	24,25,27	1.90	7 (29%)
2	DPR	m	21	2	6,7,8	0.81	0	7,8,10	1.22	1 (14%)
2	U2X	m	23	2	20,20,21	2.22	4 (20%)	24,25,27	1.90	7 (29%)
2	DPR	p	21	2	6,7,8	0.80	0	7,8,10	1.21	1 (14%)
2	U2X	p	23	2	20,20,21	2.22	5 (25%)	24,25,27	1.90	7 (29%)
2	DPR	s	21	2	6,7,8	0.80	0	7,8,10	1.22	1 (14%)
2	U2X	s	23	2	20,20,21	2.22	4 (20%)	24,25,27	1.90	7 (29%)
2	DPR	v	21	2	6,7,8	0.80	0	7,8,10	1.22	1 (14%)
2	U2X	v	23	2	20,20,21	2.23	4 (20%)	24,25,27	1.90	7 (29%)

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
4	OAS	C	30	4	-	0/5/7/9	0/0/0/0
4	OAS	F	30	4	-	0/2/4/9	0/0/0/0
4	OAS	H	30	4	-	1/5/7/9	0/0/0/0
4	OAS	J	30	4	-	0/2/4/9	0/0/0/0
4	OAS	N	30	4	-	0/2/4/9	0/0/0/0
4	OAS	Q	30	4	-	0/2/4/9	0/0/0/0
4	OAS	T	30	4	-	0/5/7/9	0/0/0/0
4	OAS	W	30	4	-	0/5/7/9	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DPR	a	21	2	-	0/0/9/11	0/1/1/1
2	U2X	a	23	2	-	0/9/19/21	0/2/2/2
2	DPR	b	21	2	-	0/0/9/11	0/1/1/1
2	U2X	b	23	2	-	0/9/19/21	0/2/2/2
2	DPR	e	21	2	-	0/0/9/11	0/1/1/1
2	U2X	e	23	2	-	0/9/19/21	0/2/2/2
2	DPR	i	21	2	-	0/0/9/11	0/1/1/1
2	U2X	i	23	2	-	0/9/19/21	0/2/2/2
2	DPR	m	21	2	-	0/0/9/11	0/1/1/1
2	U2X	m	23	2	-	0/9/19/21	0/2/2/2
2	DPR	p	21	2	-	0/0/9/11	0/1/1/1
2	U2X	p	23	2	-	0/9/19/21	0/2/2/2
2	DPR	s	21	2	-	0/0/9/11	0/1/1/1
2	U2X	s	23	2	-	0/9/19/21	0/2/2/2
2	DPR	v	21	2	-	0/0/9/11	0/1/1/1
2	U2X	v	23	2	-	0/9/19/21	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	23	U2X	CB-CA	-2.01	1.49	1.53
2	p	23	U2X	CB-CA	-2.00	1.49	1.53
4	J	30	OAS	CA-C	2.02	1.52	1.50
4	H	30	OAS	CA-C	2.04	1.52	1.50
4	C	30	OAS	CA-C	2.05	1.52	1.50
4	Q	30	OAS	CA-C	2.10	1.53	1.50
2	e	23	U2X	C4-C3	2.17	1.58	1.52
2	i	23	U2X	C4-C3	2.18	1.58	1.52
2	b	23	U2X	C4-C3	2.18	1.58	1.52
2	v	23	U2X	C4-C3	2.19	1.58	1.52
2	a	23	U2X	C4-C3	2.19	1.58	1.52
2	m	23	U2X	C4-C3	2.19	1.58	1.52
2	s	23	U2X	C4-C3	2.20	1.58	1.52
2	p	23	U2X	C4-C3	2.20	1.58	1.52
2	i	23	U2X	CE1-CZ	2.47	1.43	1.38
2	p	23	U2X	CE1-CZ	2.47	1.43	1.38
2	s	23	U2X	CE1-CZ	2.47	1.43	1.38
2	a	23	U2X	CE1-CZ	2.47	1.43	1.38
2	v	23	U2X	CE1-CZ	2.48	1.43	1.38
2	b	23	U2X	CE1-CZ	2.48	1.43	1.38
2	e	23	U2X	CE1-CZ	2.49	1.43	1.38
2	m	23	U2X	CE1-CZ	2.50	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	v	23	U2X	CE1-CD1	4.20	1.46	1.38
2	s	23	U2X	CE1-CD1	4.22	1.46	1.38
2	m	23	U2X	CE1-CD1	4.23	1.46	1.38
2	a	23	U2X	CE1-CD1	4.24	1.46	1.38
2	b	23	U2X	CE1-CD1	4.24	1.46	1.38
2	e	23	U2X	CE1-CD1	4.25	1.46	1.38
2	p	23	U2X	CE1-CD1	4.26	1.46	1.38
2	i	23	U2X	CE1-CD1	4.26	1.46	1.38
2	e	23	U2X	CE2-CD2	7.24	1.51	1.38
2	p	23	U2X	CE2-CD2	7.25	1.51	1.38
2	m	23	U2X	CE2-CD2	7.26	1.51	1.38
2	a	23	U2X	CE2-CD2	7.27	1.51	1.38
2	i	23	U2X	CE2-CD2	7.29	1.51	1.38
2	s	23	U2X	CE2-CD2	7.30	1.51	1.38
2	v	23	U2X	CE2-CD2	7.30	1.51	1.38
2	b	23	U2X	CE2-CD2	7.32	1.51	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	23	U2X	C1-C2-C3	-2.87	106.92	112.19
2	i	23	U2X	C1-C2-C3	-2.86	106.94	112.19
2	e	23	U2X	C1-C2-C3	-2.85	106.95	112.19
2	p	23	U2X	C1-C2-C3	-2.85	106.96	112.19
2	a	23	U2X	C1-C2-C3	-2.85	106.96	112.19
2	v	23	U2X	C1-C2-C3	-2.85	106.97	112.19
2	s	23	U2X	C1-C2-C3	-2.85	106.97	112.19
2	m	23	U2X	C1-C2-C3	-2.84	106.98	112.19
2	v	23	U2X	C5-C4-C3	-2.41	107.78	112.19
2	a	23	U2X	C5-C4-C3	-2.40	107.80	112.19
2	p	23	U2X	C5-C4-C3	-2.40	107.80	112.19
2	b	23	U2X	C5-C4-C3	-2.39	107.80	112.19
2	m	23	U2X	C5-C4-C3	-2.39	107.81	112.19
2	e	23	U2X	C5-C4-C3	-2.38	107.82	112.19
2	s	23	U2X	C5-C4-C3	-2.38	107.82	112.19
2	i	23	U2X	C5-C4-C3	-2.38	107.83	112.19
2	m	21	DPR	O-C-CA	-2.27	119.86	125.15
2	e	21	DPR	O-C-CA	-2.27	119.86	125.15
2	a	21	DPR	O-C-CA	-2.26	119.87	125.15
2	b	21	DPR	O-C-CA	-2.26	119.88	125.15
2	s	21	DPR	O-C-CA	-2.26	119.88	125.15
2	i	21	DPR	O-C-CA	-2.25	119.89	125.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	v	21	DPR	O-C-CA	-2.25	119.91	125.15
2	p	21	DPR	O-C-CA	-2.25	119.91	125.15
2	v	23	U2X	CD2-CG-CD1	2.14	121.56	118.16
2	e	23	U2X	CD2-CG-CD1	2.15	121.58	118.16
2	m	23	U2X	CD2-CG-CD1	2.16	121.58	118.16
2	a	23	U2X	CD2-CG-CD1	2.16	121.59	118.16
2	p	23	U2X	CD2-CG-CD1	2.17	121.60	118.16
2	i	23	U2X	CD2-CG-CD1	2.18	121.62	118.16
2	s	23	U2X	CD2-CG-CD1	2.19	121.63	118.16
2	b	23	U2X	CD2-CG-CD1	2.20	121.64	118.16
2	e	23	U2X	OH-C7-C3	2.81	114.25	107.81
2	v	23	U2X	OH-C7-C3	2.81	114.25	107.81
2	i	23	U2X	OH-C7-C3	2.81	114.25	107.81
2	s	23	U2X	OH-C7-C3	2.82	114.26	107.81
2	a	23	U2X	OH-C7-C3	2.82	114.27	107.81
2	m	23	U2X	OH-C7-C3	2.83	114.29	107.81
2	p	23	U2X	OH-C7-C3	2.84	114.30	107.81
2	b	23	U2X	OH-C7-C3	2.84	114.31	107.81
2	p	23	U2X	CG-CB-CA	2.84	120.02	114.29
2	s	23	U2X	CG-CB-CA	2.84	120.03	114.29
2	a	23	U2X	CG-CB-CA	2.85	120.05	114.29
2	m	23	U2X	CG-CB-CA	2.85	120.05	114.29
2	b	23	U2X	CG-CB-CA	2.86	120.06	114.29
2	v	23	U2X	CG-CB-CA	2.86	120.07	114.29
2	e	23	U2X	CG-CB-CA	2.86	120.07	114.29
2	i	23	U2X	CG-CB-CA	2.86	120.07	114.29
2	p	23	U2X	C4-C3-C7	3.35	118.32	111.42
2	a	23	U2X	C4-C3-C7	3.35	118.33	111.42
2	m	23	U2X	C4-C3-C7	3.35	118.34	111.42
2	v	23	U2X	C4-C3-C7	3.36	118.34	111.42
2	b	23	U2X	C4-C3-C7	3.36	118.34	111.42
2	e	23	U2X	C4-C3-C7	3.36	118.35	111.42
2	i	23	U2X	C4-C3-C7	3.37	118.36	111.42
2	s	23	U2X	C4-C3-C7	3.37	118.37	111.42
2	b	23	U2X	C2-C3-C7	4.93	121.59	111.42
2	s	23	U2X	C2-C3-C7	4.95	121.63	111.42
2	a	23	U2X	C2-C3-C7	4.95	121.63	111.42
2	v	23	U2X	C2-C3-C7	4.95	121.63	111.42
2	i	23	U2X	C2-C3-C7	4.95	121.64	111.42
2	p	23	U2X	C2-C3-C7	4.96	121.65	111.42
2	e	23	U2X	C2-C3-C7	4.96	121.66	111.42
2	m	23	U2X	C2-C3-C7	4.97	121.66	111.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	30	OAS	C1A-OG-CB-CA

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	30	OAS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 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	$\# Z > 2$
5	NAG	A	501	1	14,14,15	0.45	0	15,19,21	0.41	0
5	NAG	A	502	1	14,14,15	0.26	0	15,19,21	0.45	0
5	NAG	A	503	1	14,14,15	0.20	0	15,19,21	0.48	0
5	NAG	A	504	1	14,14,15	0.19	0	15,19,21	0.46	0
5	NAG	B	501	1	14,14,15	0.22	0	15,19,21	0.46	0
5	NAG	B	502	1	14,14,15	0.34	0	15,19,21	1.34	1 (6%)
5	NAG	E	501	1	14,14,15	0.27	0	15,19,21	0.44	0
5	NAG	E	502	1	14,14,15	0.25	0	15,19,21	0.48	0
5	NAG	I	501	1	14,14,15	0.27	0	15,19,21	0.55	0
5	NAG	I	502	1	14,14,15	0.36	0	15,19,21	0.49	0
5	NAG	I	503	1	14,14,15	0.22	0	15,19,21	0.46	0
5	NAG	I	504	1	14,14,15	0.51	0	15,19,21	0.37	0
5	NAG	M	501	1	14,14,15	0.26	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	P	501	1	14,14,15	0.23	0	15,19,21	0.39	0
5	NAG	P	502	1	14,14,15	0.32	0	15,19,21	0.54	0
5	NAG	S	501	1	14,14,15	0.23	0	15,19,21	0.45	0
5	NAG	S	502	1	14,14,15	0.50	0	15,19,21	0.86	1 (6%)
5	NAG	S	503	1	14,14,15	0.27	0	15,19,21	0.42	0
5	NAG	V	501	1	14,14,15	0.34	0	15,19,21	0.42	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
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	NAG	B	502	1	-	0/6/23/26	0/1/1/1
5	NAG	E	501	1	-	0/6/23/26	0/1/1/1
5	NAG	E	502	1	-	0/6/23/26	0/1/1/1
5	NAG	I	501	1	-	0/6/23/26	0/1/1/1
5	NAG	I	502	1	-	0/6/23/26	0/1/1/1
5	NAG	I	503	1	-	0/6/23/26	0/1/1/1
5	NAG	I	504	1	-	0/6/23/26	0/1/1/1
5	NAG	M	501	1	-	0/6/23/26	0/1/1/1
5	NAG	P	501	1	-	0/6/23/26	0/1/1/1
5	NAG	P	502	1	-	0/6/23/26	0/1/1/1
5	NAG	S	501	1	-	0/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	S	503	1	-	0/6/23/26	0/1/1/1
5	NAG	V	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	502	NAG	C1-C2-N2	2.17	114.20	110.49
5	B	502	NAG	C1-O5-C5	4.24	118.01	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	NAG	2	0
5	A	502	NAG	3	0
5	A	503	NAG	1	0
5	A	504	NAG	2	0
5	B	501	NAG	3	0
5	B	502	NAG	7	0
5	E	501	NAG	1	0
5	E	502	NAG	1	0
5	I	501	NAG	6	0
5	I	504	NAG	3	0
5	M	501	NAG	1	0
5	P	501	NAG	2	0
5	P	502	NAG	3	0
5	S	501	NAG	2	0
5	S	502	NAG	11	0
5	V	501	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	333/352 (94%)	0.54	32 (9%) 9 7	119, 153, 203, 222	0
1	B	342/352 (97%)	0.58	42 (12%) 5 5	105, 174, 268, 299	0
1	E	329/352 (93%)	0.68	47 (14%) 3 3	141, 205, 256, 283	0
1	I	341/352 (96%)	0.38	28 (8%) 12 10	120, 166, 210, 232	0
1	M	339/352 (96%)	0.56	40 (11%) 5 5	122, 188, 245, 262	0
1	P	338/352 (96%)	0.54	33 (9%) 8 7	104, 170, 241, 263	0
1	S	339/352 (96%)	0.54	26 (7%) 14 11	123, 177, 252, 283	0
1	V	338/352 (96%)	0.58	31 (9%) 10 8	122, 180, 263, 301	0
2	a	24/28 (85%)	0.37	2 (8%) 12 10	141, 188, 204, 208	0
2	b	24/28 (85%)	0.29	1 (4%) 37 27	161, 195, 225, 229	0
2	e	24/28 (85%)	0.15	1 (4%) 37 27	171, 198, 220, 223	0
2	i	24/28 (85%)	0.12	1 (4%) 37 27	140, 189, 200, 204	0
2	m	24/28 (85%)	0.37	2 (8%) 12 10	171, 209, 228, 233	0
2	p	24/28 (85%)	0.38	2 (8%) 12 10	118, 160, 181, 188	0
2	s	24/28 (85%)	0.34	2 (8%) 12 10	149, 202, 226, 231	0
2	v	24/28 (85%)	0.30	4 (16%) 2 2	170, 213, 220, 221	0
3	D	210/210 (100%)	1.29	52 (24%) 1 1	106, 227, 332, 347	0
3	G	210/210 (100%)	1.34	51 (24%) 1 1	172, 252, 328, 358	0
3	K	210/210 (100%)	2.78	84 (40%) 0 0	210, 340, 366, 371	0
3	L	210/210 (100%)	0.60	30 (14%) 3 3	146, 230, 276, 302	0
3	O	210/210 (100%)	1.23	55 (26%) 1 1	193, 256, 292, 314	0
3	R	210/210 (100%)	1.29	50 (23%) 1 1	181, 250, 340, 377	0
3	U	210/210 (100%)	0.73	33 (15%) 2 2	117, 227, 317, 334	0
3	X	210/210 (100%)	1.45	68 (32%) 0 0	185, 248, 303, 317	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9	
4	C	219/220 (99%)	1.04	51 (23%)	11	102, 188, 337, 353	0
4	F	219/220 (99%)	0.99	52 (23%)	11	189, 240, 283, 314	0
4	H	219/220 (99%)	0.65	41 (18%)	11	144, 198, 268, 280	0
4	J	219/220 (99%)	1.82	76 (34%)	00	205, 303, 380, 398	0
4	N	219/220 (99%)	1.34	57 (26%)	11	189, 240, 282, 300	0
4	Q	219/220 (99%)	0.90	47 (21%)	11	179, 241, 285, 310	0
4	T	219/220 (99%)	1.10	46 (21%)	11	125, 212, 311, 338	0
4	W	219/220 (99%)	1.17	59 (26%)	11	170, 232, 271, 292	0
All	All	6323/6480 (97%)	0.91	1146 (18%)	11	102, 208, 323, 398	0

All (1146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	197	THR	28.7
3	K	144	ALA	26.7
3	K	136	LEU	26.5
4	J	179	SER	23.6
3	K	115	VAL	22.6
3	R	149	LYS	17.7
3	D	193	ALA	17.2
4	J	11	LEU	16.4
3	K	175	LEU	16.0
3	K	145	LYS	15.2
3	K	34	ALA	15.2
3	U	181	LEU	14.4
3	G	150	VAL	14.4
4	T	211	VAL	14.0
3	R	150	VAL	13.4
3	G	181	LEU	13.3
4	J	109	VAL	13.2
1	V	459	GLY	13.2
3	K	21	ILE	13.0
3	K	177	SER	13.0
4	N	184	VAL	12.7
3	K	73	LEU	12.7
4	F	179	SER	12.7
3	K	19	VAL	12.6
4	C	180	SER	12.4
1	P	406	THR	12.4

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Mol	Chain	Res	Type	RSRZ
3	D	209	PHE	12.2
4	F	69	ILE	11.9
3	K	135	LEU	11.8
4	J	147	PRO	11.7
1	M	285	ILE	11.6
4	T	161	SER	11.5
1	E	453	ILE	11.4
3	G	132	VAL	11.4
1	A	359	ILE	11.0
3	D	181	LEU	10.7
3	O	11	VAL	10.7
3	X	132	VAL	10.4
3	O	104	LEU	10.2
3	D	150	VAL	10.1
3	G	149	LYS	10.1
4	T	126	PRO	10.1
3	K	116	PHE	10.1
4	W	211	VAL	9.9
4	J	12	LEU	9.7
3	G	116	PHE	9.5
1	V	359	ILE	9.5
3	D	135	LEU	9.5
1	M	359	ILE	9.4
3	G	131	SER	9.4
3	O	192	TYR	9.4
3	K	161	GLU	9.4
3	G	25	ALA	9.3
3	G	192	TYR	9.3
4	N	129	LYS	9.3
3	K	134	CYS	9.2
1	S	359	ILE	9.2
4	W	119	PRO	9.1
4	F	129	LYS	9.0
4	N	114	ALA	9.0
4	C	211	VAL	8.9
4	Q	111	VAL	8.9
3	K	20	THR	8.9
3	X	186	TYR	8.9
3	G	133	VAL	8.8
3	X	131	SER	8.8
4	F	180	SER	8.8
3	O	131	SER	8.7

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Mol	Chain	Res	Type	RSRZ
1	E	286	VAL	8.7
3	L	181	LEU	8.7
1	B	408	SER	8.7
3	K	204	PRO	8.6
3	O	51	ALA	8.6
3	R	116	PHE	8.5
1	M	286	VAL	8.5
3	D	144	ALA	8.4
3	D	192	TYR	8.4
4	N	112	SER	8.3
4	Q	140	CYS	8.3
4	J	69	ILE	8.2
1	E	452	LEU	8.2
4	C	184	VAL	8.2
3	K	14	SER	8.1
3	R	181	LEU	8.1
1	E	284	ILE	8.1
4	W	69	ILE	8.0
3	D	134	CYS	7.9
4	J	178	LEU	7.9
3	G	47	VAL	7.9
1	E	285	ILE	7.8
4	J	9	ALA	7.7
3	D	152	ASN	7.7
3	X	117	ILE	7.7
3	R	133	VAL	7.7
1	E	283	ASN	7.7
4	W	112	SER	7.6
4	J	180	SER	7.6
3	X	133	VAL	7.6
3	K	196	VAL	7.6
3	K	203	SER	7.5
1	S	338	TRP	7.4
3	X	193	ALA	7.4
3	K	133	VAL	7.3
4	W	29	LEU	7.3
3	X	62	PHE	7.2
3	X	194	CYS	7.2
3	R	134	CYS	7.2
4	C	138	LEU	7.2
3	R	193	ALA	7.2
4	N	18	LEU	7.2

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Mol	Chain	Res	Type	RSRZ
3	K	33	LEU	7.1
4	F	111	VAL	7.1
4	N	130	SER	7.0
4	N	179	SER	7.0
3	D	149	LYS	7.0
3	K	147	GLN	7.0
1	P	453	ILE	7.0
3	K	82	ASP	7.0
3	U	209	PHE	6.9
4	C	140	CYS	6.9
3	K	180	THR	6.9
3	O	142	ARG	6.9
4	J	110	THR	6.9
3	G	193	ALA	6.9
3	R	180	THR	6.9
4	N	111	VAL	6.8
4	J	33	TYR	6.8
4	N	160	THR	6.8
3	X	207	LYS	6.8
4	C	185	PRO	6.8
3	K	46	LEU	6.7
4	W	18	LEU	6.7
1	S	286	VAL	6.7
3	X	181	LEU	6.7
3	D	205	VAL	6.7
3	U	17	ASP	6.7
1	E	258	GLN	6.7
3	G	191	VAL	6.6
3	O	50	ALA	6.6
4	F	48	ILE	6.6
3	K	47	VAL	6.6
4	J	18	LEU	6.6
1	B	453	ILE	6.6
4	N	82	LEU	6.6
3	K	113	PRO	6.6
3	R	86	TYR	6.6
4	F	141	LEU	6.5
4	J	194	TYR	6.5
4	F	93	ALA	6.5
1	P	284	ILE	6.5
4	Q	29	LEU	6.4
1	V	93	PHE	6.4

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Mol	Chain	Res	Type	RSRZ
4	F	29	LEU	6.4
3	D	25	ALA	6.4
4	C	183	THR	6.4
4	Q	38	ARG	6.4
1	M	259	LEU	6.4
4	W	67	VAL	6.4
4	H	54	ASN	6.4
3	K	181	LEU	6.3
3	U	113	PRO	6.3
4	F	142	VAL	6.3
1	M	473	GLY	6.3
4	W	160	THR	6.3
4	C	181	VAL	6.3
1	A	286	VAL	6.3
3	O	12	SER	6.2
1	A	284	ILE	6.2
3	X	76	SER	6.2
3	G	87	TYR	6.2
4	Q	179	SER	6.2
4	C	139	GLY	6.2
4	T	110	THR	6.2
1	E	454	LEU	6.2
3	K	205	VAL	6.2
4	W	126	PRO	6.2
3	G	12	SER	6.1
4	J	166	PHE	6.1
4	J	164	HIS	6.1
4	J	35	SER	6.1
4	J	123	PRO	6.1
4	Q	27	GLU	6.1
1	M	284	ILE	6.1
3	R	201	LEU	6.1
4	J	129	LYS	6.1
4	F	181	VAL	6.1
1	A	452	LEU	6.1
1	M	452	LEU	6.1
1	V	338	TRP	6.1
1	S	259	LEU	6.0
3	K	146	VAL	6.0
4	F	67	VAL	6.0
3	L	192	TYR	6.0
4	W	121	VAL	6.0

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Mol	Chain	Res	Type	RSRZ
3	K	174	SER	6.0
3	U	151	ASP	5.9
3	K	13	ALA	5.9
4	C	11	LEU	5.9
4	J	130	SER	5.9
4	H	189	LEU	5.9
1	I	286	VAL	5.9
3	X	41	GLY	5.9
1	B	359	ILE	5.9
3	L	115	VAL	5.9
4	C	18	LEU	5.9
3	K	25	ALA	5.9
3	K	165	GLU	5.9
4	N	126	PRO	5.9
4	Q	37	VAL	5.8
3	O	29	ILE	5.8
3	L	116	PHE	5.8
3	R	135	LEU	5.8
1	V	452	LEU	5.8
3	G	11	VAL	5.8
3	X	29	ILE	5.8
4	N	110	THR	5.8
1	E	349	LEU	5.8
1	M	349	LEU	5.8
1	P	452	LEU	5.7
3	D	201	LEU	5.7
3	O	4	MET	5.7
3	O	86	TYR	5.7
3	X	168	SER	5.7
4	H	150	VAL	5.7
4	C	194	TYR	5.7
3	R	205	VAL	5.7
3	O	54	LEU	5.7
3	K	154	LEU	5.7
3	X	36	TYR	5.7
3	G	32	TYR	5.7
3	G	196	VAL	5.7
3	G	151	ASP	5.6
2	a	27	VAL	5.6
3	G	13	ALA	5.6
1	B	259	LEU	5.6
4	J	137	ALA	5.6

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Mol	Chain	Res	Type	RSRZ
4	W	37	VAL	5.6
1	S	414	ILE	5.6
4	J	71	LEU	5.6
4	H	138	LEU	5.5
3	X	192	TYR	5.5
3	G	118	PHE	5.5
1	M	338	TRP	5.5
1	I	287	GLN	5.4
3	D	131	SER	5.4
1	B	338	TRP	5.4
3	K	87	TYR	5.4
4	J	34	TRP	5.4
3	R	196	VAL	5.4
1	P	359	ILE	5.4
1	V	259	LEU	5.4
4	N	136	ALA	5.4
3	X	148	TRP	5.4
4	T	109	VAL	5.4
4	J	59	TYR	5.4
4	J	165	THR	5.4
4	N	198	VAL	5.4
4	F	150	VAL	5.4
3	R	25	ALA	5.3
1	I	359	ILE	5.3
3	G	86	TYR	5.3
4	N	69	ILE	5.3
3	L	133	VAL	5.3
1	A	290	GLU	5.3
4	W	110	THR	5.3
3	O	132	VAL	5.3
4	T	9	ALA	5.3
4	Q	35	SER	5.3
3	D	180	THR	5.3
4	W	111	VAL	5.3
4	H	90	TYR	5.2
4	C	35	SER	5.2
4	T	29	LEU	5.2
1	M	77	THR	5.2
1	B	242	VAL	5.2
3	K	15	VAL	5.2
1	B	258	GLN	5.2
4	N	107	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	E	359	ILE	5.1
4	W	161	SER	5.1
4	C	123	PRO	5.1
4	T	186	SER	5.1
4	T	18	LEU	5.1
3	K	155	GLN	5.1
4	J	210	LYS	5.1
1	M	361	PHE	5.1
3	O	41	GLY	5.1
4	T	129	LYS	5.1
3	K	150	VAL	5.0
3	D	198	HIS	5.0
1	M	488	VAL	5.0
3	U	142	ARG	5.0
1	V	253	PRO	5.0
3	L	135	LEU	5.0
4	J	149	PRO	5.0
1	V	409	ILE	5.0
4	C	82	LEU	4.9
3	R	207	LYS	4.9
1	V	272	ILE	4.9
4	H	11	LEU	4.9
4	F	109	VAL	4.9
3	K	114	SER	4.9
4	T	209	LYS	4.9
3	L	35	TRP	4.9
3	D	153	ALA	4.9
4	C	122	PHE	4.8
1	A	285	ILE	4.8
4	J	148	GLU	4.8
1	I	285	ILE	4.8
1	M	50	THR	4.8
4	N	71	LEU	4.8
3	R	151	ASP	4.8
3	K	194	CYS	4.7
4	W	96	SER	4.7
3	K	62	PHE	4.7
3	O	144	ALA	4.7
4	T	82	LEU	4.7
3	O	210	ASN	4.7
3	K	206	THR	4.7
1	I	407	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	453	ILE	4.7
1	P	454	LEU	4.7
4	J	87	THR	4.7
3	D	136	LEU	4.7
4	T	25	TYR	4.7
4	W	132	SER	4.7
3	K	211	ARG	4.7
2	p	17	GLY	4.7
1	V	453	ILE	4.7
3	R	62	PHE	4.7
3	R	47	VAL	4.7
4	W	71	LEU	4.7
3	D	196	VAL	4.6
3	U	193	ALA	4.6
4	Q	36	TRP	4.6
1	P	338	TRP	4.6
3	D	147	GLN	4.6
3	O	103	LYS	4.6
4	T	214	LYS	4.6
3	R	87	TYR	4.6
4	J	29	LEU	4.6
1	B	407	ALA	4.6
4	J	8	GLY	4.6
1	P	471	GLY	4.5
3	R	24	ARG	4.5
3	R	19	VAL	4.5
4	W	213	PRO	4.5
3	X	51	ALA	4.5
4	H	10	GLY	4.5
4	J	108	LEU	4.5
1	P	58	ALA	4.5
3	R	132	VAL	4.5
4	T	34	TRP	4.5
1	V	284	ILE	4.5
3	O	118	PHE	4.5
4	H	110	THR	4.5
1	V	473	GLY	4.5
3	O	130	ALA	4.5
3	D	115	VAL	4.5
4	J	27	GLU	4.5
4	J	195	ILE	4.5
1	A	492	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	35	SER	4.4
3	K	149	LYS	4.4
4	C	108	LEU	4.4
4	W	82	LEU	4.4
3	U	150	VAL	4.4
4	T	56	SER	4.4
1	M	260	LEU	4.4
3	G	33	LEU	4.4
3	U	192	TYR	4.4
4	C	186	SER	4.4
4	F	100(C)	PHE	4.4
4	J	86	ASP	4.3
4	N	11	LEU	4.3
4	Q	110	THR	4.3
3	G	117	ILE	4.3
3	R	152	ASN	4.3
1	V	258	GLN	4.3
3	L	78	LEU	4.3
3	L	144	ALA	4.3
3	O	62	PHE	4.3
2	s	27	VAL	4.3
4	N	185	PRO	4.3
1	V	390	LEU	4.3
1	B	86	MET	4.3
3	D	86	TYR	4.3
1	B	281	VAL	4.3
4	W	207	VAL	4.3
4	T	10	GLY	4.2
4	H	109	VAL	4.2
4	W	12	LEU	4.2
3	G	135	LEU	4.2
4	Q	80	LEU	4.2
1	E	242	VAL	4.2
1	A	287	GLN	4.2
1	M	254	VAL	4.2
4	H	18	LEU	4.2
4	H	17	THR	4.2
1	B	452	LEU	4.1
3	L	47	VAL	4.1
3	O	10	PHE	4.1
3	G	161	GLU	4.1
1	A	483	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
4	J	189	LEU	4.1
1	E	357	ASN	4.1
1	S	82	GLN	4.1
1	S	285	ILE	4.1
4	F	27	GLU	4.1
4	Q	69	ILE	4.1
1	E	259	LEU	4.1
3	X	129	THR	4.1
4	W	141	LEU	4.1
4	H	80	LEU	4.1
4	W	122	PHE	4.1
3	G	134	CYS	4.0
3	G	24	ARG	4.0
1	A	338	TRP	4.0
3	K	143	GLU	4.0
4	H	213	PRO	4.0
3	X	115	VAL	4.0
3	L	134	CYS	4.0
1	I	50	THR	4.0
1	S	452	LEU	4.0
1	I	338	TRP	4.0
1	P	349	LEU	4.0
4	H	67	VAL	4.0
1	I	60	ALA	4.0
4	J	93	ALA	4.0
4	J	190	GLY	4.0
3	L	29	ILE	4.0
4	T	11	LEU	4.0
1	A	361	PHE	3.9
1	M	453	ILE	3.9
3	U	191	VAL	3.9
4	C	126	PRO	3.9
3	L	209	PHE	3.9
4	C	137	ALA	3.9
4	J	181	VAL	3.9
4	J	82	LEU	3.9
1	S	453	ILE	3.9
3	L	118	PHE	3.9
1	P	283	ASN	3.9
3	X	11	VAL	3.9
3	G	62	PHE	3.9
4	Q	91	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	420	ILE	3.9
3	R	153	ALA	3.9
4	C	182	VAL	3.9
4	N	4	LEU	3.9
4	Q	126	PRO	3.9
3	K	148	TRP	3.9
4	J	73	MET	3.9
1	P	258	GLN	3.9
1	B	468	PHE	3.9
4	T	100(C)	PHE	3.9
1	B	45	TRP	3.9
1	E	301	ASN	3.9
1	I	284	ILE	3.8
3	R	17	ASP	3.8
1	A	349	LEU	3.8
3	G	179	LEU	3.8
3	U	196	VAL	3.8
4	N	146	PHE	3.8
3	U	180	THR	3.8
1	B	333	VAL	3.8
1	A	468	PHE	3.8
3	L	33	LEU	3.8
3	R	92	ILE	3.8
3	O	35	TRP	3.8
4	T	189	LEU	3.8
3	D	33	LEU	3.8
4	C	20	LEU	3.8
1	S	58	ALA	3.8
4	J	10	GLY	3.7
4	H	137	ALA	3.7
4	N	207	VAL	3.7
4	C	38	ARG	3.7
4	J	102	PRO	3.7
3	U	161	GLU	3.7
4	N	127	SER	3.7
3	K	132	VAL	3.7
3	R	194	CYS	3.7
4	N	12	LEU	3.7
4	H	108	LEU	3.7
3	R	128	GLY	3.7
4	F	130	SER	3.7
1	A	451	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
4	N	152	VAL	3.7
4	W	124	LEU	3.7
4	Q	11	LEU	3.7
3	K	190	LYS	3.7
1	V	349	LEU	3.7
3	K	163	VAL	3.7
3	L	149	LYS	3.7
3	O	191	VAL	3.7
3	O	1	ASP	3.6
4	J	167	PRO	3.6
4	N	142	VAL	3.6
3	X	104	LEU	3.6
2	v	27	VAL	3.6
3	K	83	PHE	3.6
4	N	67	VAL	3.6
3	D	116	PHE	3.6
1	M	217	TYR	3.6
3	X	77	SER	3.6
4	F	110	THR	3.6
1	V	374	HIS	3.6
4	W	80	LEU	3.6
1	M	272	ILE	3.6
1	M	261	LEU	3.6
3	R	147	GLN	3.6
4	J	45	LEU	3.6
4	N	14	PRO	3.6
3	D	133	VAL	3.6
1	P	100	MET	3.6
4	Q	214	LYS	3.5
4	W	129	LYS	3.5
1	V	285	ILE	3.5
3	K	193	ALA	3.5
3	O	21	ILE	3.5
4	F	205	THR	3.5
1	B	284	ILE	3.5
1	A	288	LEU	3.5
1	B	339	ASN	3.5
3	U	118	PHE	3.5
3	O	84	ALA	3.5
3	L	130	ALA	3.5
4	Q	20	LEU	3.5
1	P	213	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	346	VAL	3.5
3	X	102	THR	3.5
3	K	110	VAL	3.5
3	D	82	ASP	3.5
3	R	161	GLU	3.5
1	E	282	LYS	3.5
3	K	162	SER	3.5
4	F	91	PHE	3.5
4	W	125	ALA	3.5
1	I	454	LEU	3.4
1	P	285	ILE	3.4
1	S	381	GLU	3.4
4	T	59	TYR	3.4
4	F	34	TRP	3.4
3	R	136	LEU	3.4
3	O	196	VAL	3.4
3	D	124	GLN	3.4
3	O	194	CYS	3.4
4	H	198	VAL	3.4
3	X	33	LEU	3.4
4	W	113	SER	3.4
3	D	137	ASN	3.4
4	W	210	LYS	3.4
3	X	47	VAL	3.4
3	K	22	THR	3.4
1	S	468	PHE	3.4
4	F	18	LEU	3.4
1	B	405	GLY	3.4
1	I	335	GLY	3.3
3	D	203	SER	3.3
3	D	204	PRO	3.3
1	E	338	TRP	3.3
1	S	287	GLN	3.3
3	U	78	LEU	3.3
4	F	68	THR	3.3
4	F	87	THR	3.3
4	J	115	SER	3.3
4	C	9	ALA	3.3
3	K	126	LYS	3.3
1	P	322	SER	3.3
1	S	342	LEU	3.3
4	F	194	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
3	G	144	ALA	3.3
4	W	114	ALA	3.3
1	P	470	PRO	3.3
4	F	178	LEU	3.3
3	X	178	THR	3.3
1	B	294	ILE	3.3
3	G	141	PRO	3.3
4	Q	71	LEU	3.3
4	N	131	THR	3.2
4	W	91	PHE	3.2
4	J	193	THR	3.2
3	G	210	ASN	3.2
4	N	91	PHE	3.2
4	C	135	THR	3.2
4	J	98	TRP	3.2
2	m	26	CYS	3.2
3	R	115	VAL	3.2
4	W	140	CYS	3.2
3	R	46	LEU	3.2
4	F	213	PRO	3.2
3	O	133	VAL	3.2
4	W	154	TRP	3.2
1	A	342	LEU	3.2
1	V	408	SER	3.2
3	D	114	SER	3.2
1	I	406	THR	3.2
4	N	87	THR	3.2
3	R	183	LYS	3.2
3	X	130	ALA	3.2
3	R	117	ILE	3.2
4	C	170	LEU	3.2
3	R	1	ASP	3.2
3	K	86	TYR	3.2
1	P	468	PHE	3.2
3	O	13	ALA	3.2
4	T	137	ALA	3.2
3	L	201	LEU	3.2
3	D	117	ILE	3.2
4	T	50	GLU	3.2
1	E	83	GLU	3.1
1	E	361	PHE	3.1
3	O	122	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
4	H	126	PRO	3.1
4	W	109	VAL	3.1
4	C	124	LEU	3.1
4	C	19	SER	3.1
4	N	140	CYS	3.1
1	M	451	GLY	3.1
4	W	48	ILE	3.1
3	X	60	SER	3.1
4	Q	98	TRP	3.1
4	T	150	VAL	3.1
4	H	71	LEU	3.1
1	E	383	PHE	3.1
3	X	19	VAL	3.1
4	W	34	TRP	3.1
3	G	2	ILE	3.1
3	K	17	ASP	3.1
4	W	212	GLU	3.1
1	S	374	HIS	3.1
1	V	60	ALA	3.1
1	V	414	ILE	3.1
4	C	207	VAL	3.1
1	E	342	LEU	3.1
1	E	56	SER	3.1
4	T	154	TRP	3.0
4	H	140	CYS	3.0
4	H	190	GLY	3.0
1	S	49	ASN	3.0
3	K	10	PHE	3.0
4	H	100(C)	PHE	3.0
1	P	49	ASN	3.0
1	M	220	PRO	3.0
4	F	38	ARG	3.0
4	W	100(C)	PHE	3.0
3	O	181	LEU	3.0
4	J	158	ALA	3.0
4	N	206	LYS	3.0
3	X	167	ASP	3.0
3	O	102	THR	3.0
4	N	161	SER	3.0
3	K	80	PRO	3.0
4	W	20	LEU	3.0
1	S	361	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	49	ASN	3.0
3	K	153	ALA	3.0
4	Q	45	LEU	3.0
1	I	452	LEU	3.0
1	M	454	LEU	3.0
3	X	185	ASP	3.0
3	O	129	THR	3.0
4	T	95	ARG	3.0
4	T	213	PRO	3.0
4	J	92	CYS	3.0
4	W	152	VAL	3.0
4	N	147	PRO	3.0
3	X	187	GLU	3.0
4	J	106	GLY	3.0
4	J	111	VAL	2.9
1	V	410	GLU	2.9
1	E	350	ARG	2.9
3	D	87	TYR	2.9
3	O	79	GLN	2.9
3	K	187	GLU	2.9
1	S	242	VAL	2.9
4	F	115	SER	2.9
4	Q	34	TRP	2.9
4	Q	48	ILE	2.9
1	V	100	MET	2.9
1	E	50	THR	2.9
3	U	86	TYR	2.9
1	V	49	ASN	2.9
4	F	212	GLU	2.9
3	O	205	VAL	2.9
3	U	127	SER	2.9
3	D	200	GLY	2.9
1	M	483	LEU	2.9
3	G	31	SER	2.9
1	B	472	GLY	2.9
4	H	132	SER	2.9
4	F	95	ARG	2.9
4	Q	132	SER	2.9
3	G	105	GLU	2.9
4	H	59	TYR	2.9
4	J	187	SER	2.9
4	T	57	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
4	N	159	LEU	2.9
1	E	492	GLU	2.9
1	V	286	VAL	2.9
1	E	488	VAL	2.9
3	K	202	SER	2.9
3	R	148	TRP	2.9
1	S	390	LEU	2.9
3	R	130	ALA	2.9
3	X	61	ARG	2.9
4	Q	54	ASN	2.9
1	P	217	TYR	2.9
4	C	193	THR	2.9
4	J	48	ILE	2.9
3	O	193	ALA	2.9
4	C	179	SER	2.9
3	D	78	LEU	2.9
1	B	349	LEU	2.8
3	G	48	ILE	2.8
4	Q	175	LEU	2.8
3	L	196	VAL	2.8
3	O	146	VAL	2.8
1	B	285	ILE	2.8
1	V	342	LEU	2.8
3	X	183	LYS	2.8
1	E	346	VAL	2.8
4	J	142	VAL	2.8
3	O	105	GLU	2.8
3	X	87	TYR	2.8
4	F	132	SER	2.8
3	L	158	ASN	2.8
1	I	349	LEU	2.8
3	R	113	PRO	2.8
3	X	46	LEU	2.8
4	Q	82	LEU	2.8
1	P	286	VAL	2.8
1	S	349	LEU	2.8
2	v	17	GLY	2.8
3	L	132	VAL	2.8
4	J	186	SER	2.8
1	A	381	GLU	2.8
1	S	272	ILE	2.8
3	G	104	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
4	N	17	THR	2.8
1	M	100	MET	2.8
3	R	179	LEU	2.8
4	J	78	PHE	2.8
1	E	381	GLU	2.8
3	L	38	GLN	2.8
3	X	134	CYS	2.8
4	J	152	VAL	2.8
3	X	118	PHE	2.8
3	G	143	GLU	2.8
4	T	184	VAL	2.8
4	C	34	TRP	2.8
4	J	91	PHE	2.8
4	T	185	PRO	2.8
4	H	69	ILE	2.8
4	T	69	ILE	2.8
3	O	85	THR	2.8
4	J	21	THR	2.8
4	H	180	SER	2.8
3	O	148	TRP	2.8
4	W	173	SER	2.7
3	U	21	ILE	2.7
3	X	149	LYS	2.7
3	L	117	ILE	2.7
3	D	182	SER	2.7
4	F	92	CYS	2.7
1	B	470	PRO	2.7
1	M	487	LYS	2.7
4	F	184	VAL	2.7
1	V	381	GLU	2.7
3	U	110	VAL	2.7
4	N	150	VAL	2.7
1	B	492	GLU	2.7
3	G	129	THR	2.7
3	O	40	PRO	2.7
1	M	342	LEU	2.7
3	O	206	THR	2.7
4	N	194	TYR	2.7
4	W	123	PRO	2.7
4	C	10	GLY	2.7
4	J	124	LEU	2.7
4	Q	108	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	V	217	TYR	2.7
4	W	11	LEU	2.7
3	G	180	THR	2.7
3	X	142	ARG	2.7
1	B	240	LYS	2.7
1	E	217	TYR	2.7
3	D	186	TYR	2.7
3	R	154	LEU	2.7
4	N	141	LEU	2.7
4	W	4	LEU	2.7
4	J	150	VAL	2.7
3	U	117	ILE	2.7
4	C	98	TRP	2.7
3	O	36	TYR	2.7
1	B	457	ASP	2.7
3	X	75	ILE	2.7
3	X	165	GLU	2.7
4	J	95	ARG	2.7
4	J	138	LEU	2.7
4	J	141	LEU	2.7
1	I	361	PHE	2.7
1	S	288	LEU	2.7
2	i	18	ARG	2.7
4	N	148	GLU	2.7
1	E	288	LEU	2.7
4	H	4	LEU	2.7
4	H	45	LEU	2.7
4	H	179	SER	2.7
3	D	47	VAL	2.7
3	K	192	TYR	2.7
3	O	117	ILE	2.7
3	K	195	GLU	2.6
4	F	214	LYS	2.6
3	X	208	SER	2.6
4	H	29	LEU	2.6
4	N	157	GLY	2.6
1	E	69	TRP	2.6
4	Q	165	THR	2.6
4	F	33	TYR	2.6
4	T	210	LYS	2.6
1	S	93	PHE	2.6
1	B	454	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
4	N	180	SER	2.6
1	B	87	GLU	2.6
3	X	94	LEU	2.6
1	B	409	ILE	2.6
3	X	198	HIS	2.6
4	W	17	THR	2.6
3	X	144	ALA	2.6
4	C	80	LEU	2.6
1	A	345	VAL	2.6
3	G	115	VAL	2.6
3	X	122	ASP	2.6
3	X	125	LEU	2.6
3	K	207	LYS	2.6
4	N	125	ALA	2.6
1	I	324	GLY	2.6
3	K	151	ASP	2.6
4	N	149	PRO	2.6
2	b	27	VAL	2.6
3	D	19	VAL	2.6
4	W	214	LYS	2.6
1	E	272	ILE	2.6
3	R	27	GLN	2.6
3	X	124	GLN	2.6
1	B	60	ALA	2.6
1	S	284	ILE	2.6
1	B	392	ASN	2.5
1	M	288	LEU	2.5
3	K	201	LEU	2.5
3	D	145	LYS	2.5
1	I	345	VAL	2.5
3	R	186	TYR	2.5
1	E	93	PHE	2.5
4	F	121	VAL	2.5
4	W	162	GLY	2.5
3	G	197	THR	2.5
4	C	110	THR	2.5
4	T	183	THR	2.5
4	W	159	LEU	2.5
4	J	90	TYR	2.5
4	Q	184	VAL	2.5
3	X	182	SER	2.5
4	W	120	SER	2.5

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Mol	Chain	Res	Type	RSRZ
4	T	119	PRO	2.5
1	B	443	ILE	2.5
3	G	54	LEU	2.5
3	R	175	LEU	2.5
1	E	423	ILE	2.5
3	D	163	VAL	2.5
1	I	408	SER	2.5
3	O	190	LYS	2.5
3	U	141	PRO	2.5
1	E	477	ASP	2.5
1	E	107	ASP	2.5
3	K	118	PHE	2.5
3	K	29	ILE	2.5
1	B	486	TYR	2.5
1	A	324	GLY	2.5
4	N	70	SER	2.5
3	R	126	LYS	2.5
4	H	139	GLY	2.5
2	m	27	VAL	2.5
3	K	179	LEU	2.5
3	L	168	SER	2.5
4	T	27	GLU	2.5
1	M	253	PRO	2.4
4	Q	106	GLY	2.4
4	Q	170	LEU	2.4
4	C	69	ILE	2.4
1	M	374	HIS	2.4
1	M	52	LEU	2.4
4	Q	207	VAL	2.4
2	v	18	ARG	2.4
3	R	55	GLN	2.4
3	X	166	GLN	2.4
4	H	3	GLN	2.4
3	U	123	GLU	2.4
4	F	80	LEU	2.4
4	F	98	TRP	2.4
3	D	151	ASP	2.4
3	O	20	THR	2.4
3	U	33	LEU	2.4
4	N	124	LEU	2.4
4	F	103	TRP	2.4
4	J	140	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	Q	181	VAL	2.4
3	G	152	ASN	2.4
1	B	46	LYS	2.4
4	H	95	ARG	2.4
3	O	186	TYR	2.4
1	P	420	ILE	2.4
4	N	68	THR	2.4
4	J	126	PRO	2.4
4	F	90	TYR	2.4
4	T	194	TYR	2.4
3	G	142	ARG	2.4
1	E	287	GLN	2.4
1	S	81	PRO	2.4
4	W	198	VAL	2.4
3	K	123	GLU	2.4
3	R	2	ILE	2.4
1	B	477	ASP	2.4
1	E	468	PHE	2.4
3	K	48	ILE	2.4
3	D	177	SER	2.4
3	X	120	PRO	2.4
1	V	471	GLY	2.4
3	D	107	LYS	2.4
3	K	55	GLN	2.4
4	C	12	LEU	2.4
4	C	132	SER	2.4
3	K	1	ASP	2.4
1	I	381	GLU	2.3
1	E	91	GLU	2.3
3	X	40	PRO	2.3
4	W	50	GLU	2.3
1	I	288	LEU	2.3
4	Q	55	GLY	2.3
4	Q	97	ASN	2.3
4	Q	121	VAL	2.3
3	U	62	PHE	2.3
4	H	130	SER	2.3
4	H	111	VAL	2.3
1	E	376	PHE	2.3
2	a	18	ARG	2.3
3	U	143	GLU	2.3
1	A	271	MET	2.3

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Mol	Chain	Res	Type	RSRZ
4	J	67	VAL	2.3
4	W	68	THR	2.3
4	W	196	CYS	2.3
3	D	143	GLU	2.3
3	U	35	TRP	2.3
4	F	82	LEU	2.3
3	L	136	LEU	2.3
4	J	173	SER	2.3
1	A	259	LEU	2.3
3	U	198	HIS	2.3
4	C	136	ALA	2.3
1	M	390	LEU	2.3
3	X	73	LEU	2.3
1	P	361	PHE	2.3
4	J	100(C)	PHE	2.3
2	s	18	ARG	2.3
4	W	183	THR	2.3
4	Q	92	CYS	2.3
3	D	14	SER	2.3
3	O	168	SER	2.3
1	M	345	VAL	2.3
1	P	333	VAL	2.3
3	X	86	TYR	2.3
4	N	37	VAL	2.3
4	Q	46	GLU	2.3
1	E	105	HIS	2.3
3	X	48	ILE	2.3
4	F	126	PRO	2.3
3	O	143	GLU	2.3
1	P	342	LEU	2.3
3	D	194	CYS	2.3
4	H	181	VAL	2.3
4	C	198	VAL	2.3
1	I	492	GLU	2.3
1	P	419	ARG	2.3
3	G	126	LYS	2.3
3	G	147	GLN	2.3
3	G	166	GLN	2.3
3	O	19	VAL	2.3
3	O	94	LEU	2.3
4	W	142	VAL	2.3
1	P	405	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	X	209	PHE	2.3
1	B	78	ASP	2.3
3	X	20	THR	2.3
1	P	259	LEU	2.3
4	F	71	LEU	2.3
4	T	37	VAL	2.3
1	P	253	PRO	2.2
4	C	141	LEU	2.2
4	F	198	VAL	2.2
4	C	59	TYR	2.2
4	C	107	THR	2.2
3	X	81	GLU	2.2
3	K	35	TRP	2.2
3	O	179	LEU	2.2
4	W	81	ASN	2.2
1	I	270	VAL	2.2
4	F	189	LEU	2.2
4	N	132	SER	2.2
3	L	147	GLN	2.2
2	v	16	LEU	2.2
3	R	78	LEU	2.2
1	M	486	TYR	2.2
3	X	201	LEU	2.2
1	V	273	ARG	2.2
4	H	129	LYS	2.2
3	X	153	ALA	2.2
4	F	152	VAL	2.2
4	F	170	LEU	2.2
4	T	152	VAL	2.2
3	X	164	THR	2.2
1	E	345	VAL	2.2
1	M	381	GLU	2.2
4	Q	28	SER	2.2
4	Q	115	SER	2.2
4	N	178	LEU	2.2
1	A	351	LYS	2.2
1	S	324	GLY	2.2
3	D	127	SER	2.2
3	X	179	LEU	2.2
4	H	78	PHE	2.2
1	A	49	ASN	2.2
1	I	486	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	52	LEU	2.2
4	N	27	GLU	2.2
4	N	151	THR	2.2
3	L	163	VAL	2.2
4	F	211	VAL	2.2
4	Q	70	SER	2.2
1	A	346	VAL	2.2
4	J	80	LEU	2.2
1	M	273	ARG	2.2
4	C	195	ILE	2.2
4	C	209	LYS	2.2
4	Q	1	GLN	2.2
3	X	123	GLU	2.2
1	B	80	SER	2.2
1	P	381	GLU	2.2
3	K	24	ARG	2.2
4	J	5	GLN	2.2
4	T	143	LYS	2.2
3	X	116	PHE	2.2
4	H	91	PHE	2.2
3	K	137	ASN	2.2
4	F	131	THR	2.2
4	T	200	HIS	2.2
1	A	454	LEU	2.2
4	Q	209	LYS	2.2
1	B	79	PRO	2.1
3	G	205	VAL	2.1
3	K	208	SER	2.1
3	K	78	LEU	2.1
1	M	406	THR	2.1
3	R	158	ASN	2.1
3	D	183	LYS	2.1
3	U	144	ALA	2.1
3	X	13	ALA	2.1
4	C	73	MET	2.1
3	K	2	ILE	2.1
4	J	155	ASN	2.1
4	Q	183	THR	2.1
1	E	261	LEU	2.1
1	I	453	ILE	2.1
1	M	383	PHE	2.1
3	U	112	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
4	C	134	GLY	2.1
4	J	209	LYS	2.1
1	P	86	MET	2.1
4	T	124	LEU	2.1
4	C	214	LYS	2.1
1	I	341	THR	2.1
2	e	22	THR	2.1
4	T	48	ILE	2.1
4	W	143	LYS	2.1
1	M	416	LEU	2.1
3	R	177	SER	2.1
1	P	357	ASN	2.1
1	A	121	GLN	2.1
1	E	199	SER	2.1
1	M	274	SER	2.1
4	F	113	SER	2.1
4	N	85	ALA	2.1
1	B	49	ASN	2.1
1	E	260	LEU	2.1
1	V	250	GLY	2.1
3	O	165	GLU	2.1
3	U	201	LEU	2.1
4	C	8	GLY	2.1
4	N	48	ILE	2.1
1	A	226	LEU	2.1
1	A	482	GLU	2.1
3	D	146	VAL	2.1
4	N	29	LEU	2.1
4	T	121	VAL	2.1
1	A	93	PHE	2.1
1	B	282	LYS	2.1
3	U	25	ALA	2.1
1	I	300	ASN	2.1
4	H	97	ASN	2.1
1	E	210	PHE	2.1
4	Q	180	SER	2.1
3	O	197	THR	2.1
1	V	99	ASN	2.1
3	D	142	ARG	2.1
4	W	54	ASN	2.1
1	B	361	PHE	2.1
1	P	407	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	I	217	TYR	2.0
3	K	94	LEU	2.0
3	X	146	VAL	2.0
4	J	184	VAL	2.0
4	Q	100(C)	PHE	2.0
3	K	91	LEU	2.0
4	Q	109	VAL	2.0
3	G	26	SER	2.0
3	U	186	TYR	2.0
4	T	35	SER	2.0
4	C	189	LEU	2.0
1	E	451	GLY	2.0
4	T	111	VAL	2.0
3	G	199	GLN	2.0
1	B	406	THR	2.0
1	I	471	GLY	2.0
3	U	57	GLY	2.0
2	p	18	ARG	2.0
4	H	131	THR	2.0
4	J	196	CYS	2.0
4	T	136	ALA	2.0
3	L	205	VAL	2.0
3	D	207	LYS	2.0
4	N	121	VAL	2.0
3	L	14	SER	2.0
1	A	198	GLY	2.0
3	L	131	SER	2.0
4	W	180	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	U2X	p	23	19/20	0.80	0.37	-	106,113,127,130	0
2	DPR	b	21	7/8	0.94	0.18	-	165,166,170,173	0
2	DPR	v	21	7/8	0.95	0.39	-	170,171,176,180	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	U2X	a	23	19/20	0.85	0.44	-	130,136,145,145	0
2	U2X	v	23	19/20	0.93	0.33	-	146,156,181,182	0
2	U2X	i	23	19/20	0.86	0.43	-	133,139,150,152	0
4	OAS	F	30	6/10	0.83	0.13	-	248,273,281,281	0
4	OAS	C	30	9/10	0.92	0.28	-	155,165,179,180	0
2	DPR	i	21	7/8	0.94	0.26	-	136,137,141,144	0
2	U2X	b	23	19/20	0.81	0.39	-	131,154,176,177	0
4	OAS	Q	30	6/10	0.68	0.30	-	246,262,273,274	0
4	OAS	J	30	6/10	0.82	0.12	-	164,236,245,246	0
2	DPR	a	21	7/8	0.95	0.17	-	146,147,150,151	0
2	DPR	p	21	7/8	0.93	0.25	-	123,126,133,136	0
2	U2X	m	23	19/20	0.91	0.35	-	155,164,181,184	0
4	OAS	W	30	9/10	0.71	0.38	-	201,211,216,219	0
2	DPR	s	21	7/8	0.95	0.17	-	151,152,155,158	0
4	OAS	H	30	9/10	0.89	0.14	-	172,176,180,182	0
4	OAS	N	30	6/10	0.82	0.18	-	179,233,246,251	0
2	DPR	m	21	7/8	0.97	0.26	-	173,175,182,187	0
2	DPR	e	21	7/8	0.98	0.33	-	176,177,180,182	0
2	U2X	e	23	19/20	0.78	0.42	-	175,179,184,185	0
4	OAS	T	30	9/10	0.86	0.23	-	156,170,195,200	0
2	U2X	s	23	19/20	0.84	0.37	-	146,152,160,160	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	503	14/15	0.89	0.35	1.33	152,167,177,182	0
5	NAG	S	501	14/15	0.84	0.36	0.71	154,162,168,171	0
5	NAG	A	501	14/15	0.87	0.36	0.58	127,136,143,144	0
5	NAG	E	502	14/15	0.74	0.28	0.40	190,201,211,212	0
5	NAG	V	501	14/15	0.93	0.38	0.40	153,158,163,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	P	502	14/15	0.75	0.26	0.35	208,216,230,231	0
5	NAG	E	501	14/15	0.84	0.38	0.27	204,207,209,209	0
5	NAG	I	502	14/15	0.58	0.43	0.22	183,189,198,199	0
5	NAG	S	503	14/15	0.89	0.29	0.15	202,210,214,216	0
5	NAG	M	501	14/15	0.86	0.42	0.14	178,180,182,185	0
5	NAG	I	504	14/15	0.80	0.26	0.14	176,180,185,186	0
5	NAG	B	501	14/15	0.80	0.28	-0.09	152,161,168,170	0
5	NAG	S	502	14/15	0.86	0.18	-0.30	230,238,252,259	0
5	NAG	I	501	14/15	0.93	0.23	-0.43	161,165,172,173	0
5	NAG	P	501	14/15	0.91	0.23	-0.48	153,165,177,177	0
5	NAG	A	502	14/15	0.88	0.20	-0.69	184,189,200,200	0
5	NAG	B	502	14/15	0.86	0.12	-0.82	219,232,245,249	0
5	NAG	A	504	14/15	0.84	0.14	-	184,188,192,195	0
5	NAG	I	503	14/15	0.86	0.21	-	194,202,208,209	0

6.5 Other polymers [i](#)

There are no such residues in this entry.