



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 04:38 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

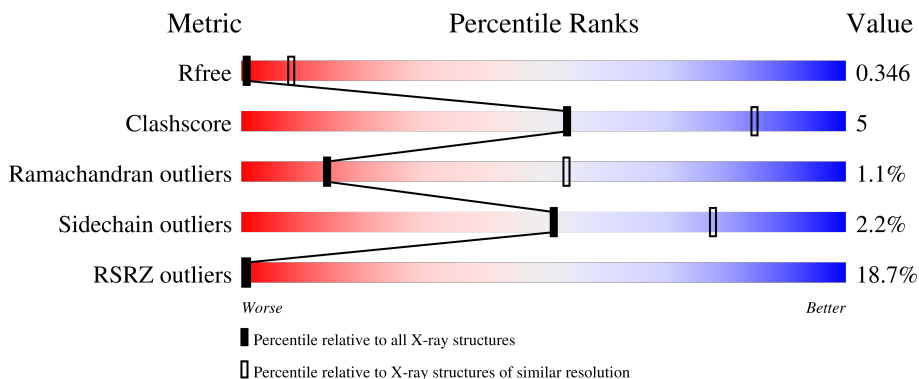
# 1 Overall quality at a glance

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.



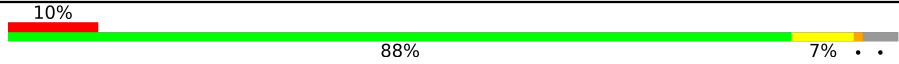
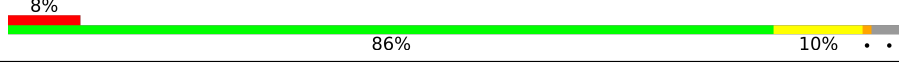
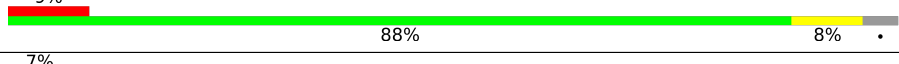
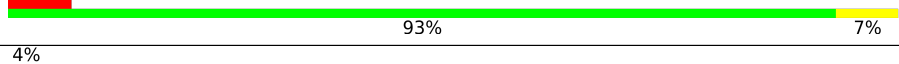
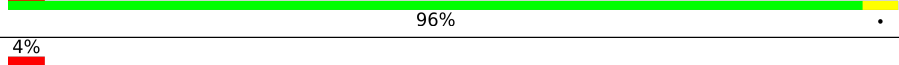
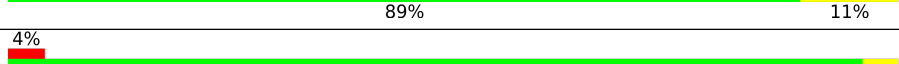
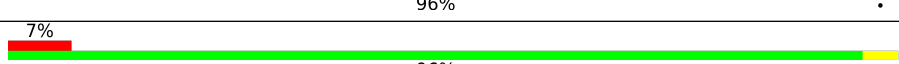
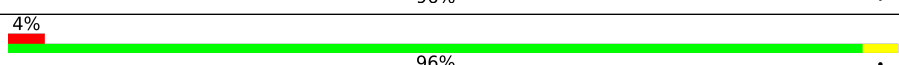
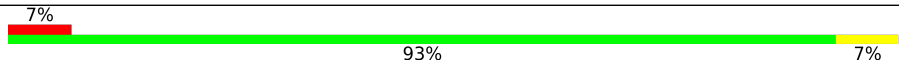
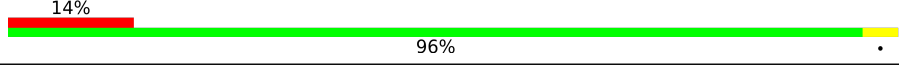

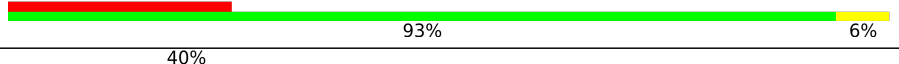
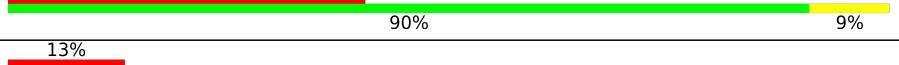
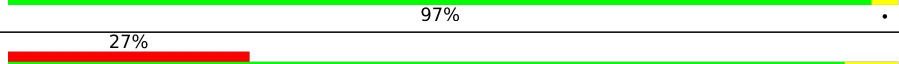
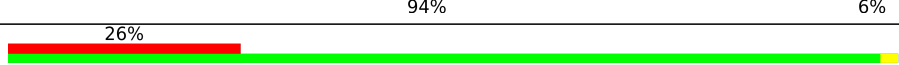
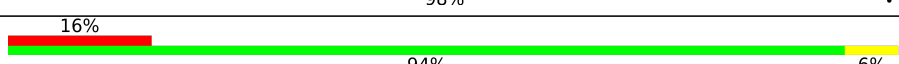
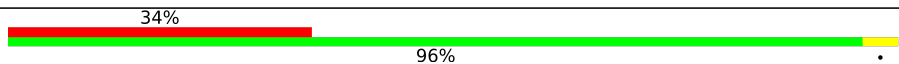


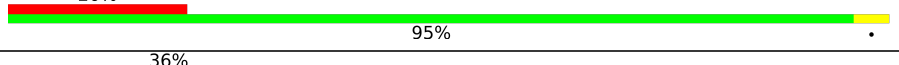





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	 9% 87% 7% 5%
1	B	352	 13% 88% 9% ..
1	E	352	 14% 87% 6% 7%
1	I	352	 9% 88% 9% ..
1	M	352	 12% 88% 8% ..

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Mol	Chain	Length	Quality of chain
1	P	352	
1	S	352	
1	V	352	
2	a	28	
2	b	28	
2	e	28	
2	i	28	
2	m	28	
2	p	28	
2	s	28	
2	v	28	
3	D	210	
3	G	210	
3	K	210	
3	L	210	
3	O	210	
3	R	210	
3	U	210	
3	X	210	
4	C	220	
4	F	220	
4	H	220	
4	J	220	
4	N	220	
4	Q	220	

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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
2	U2X	e	23	-	-	-	X
5	NAG	B	502	-	-	X	-
5	NAG	I	502	-	-	-	X
5	NAG	S	502	-	-	X	-

## 2 Entry composition [i](#)

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

- Molecule 2 is a protein called M48U1 peptide.

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

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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	C	H	N	O	S	0	0	0
			3197	1012	1585	272	323	5			
3	D	210	Total	C	H	N	O	S	0	0	0
			3196	1012	1584	272	323	5			
3	G	210	Total	C	H	N	O	S	0	0	0
			3194	1012	1582	272	323	5			
3	K	210	Total	C	H	N	O	S	0	0	0
			3195	1012	1583	272	323	5			
3	O	210	Total	C	H	N	O	S	0	0	0
			3198	1012	1586	272	323	5			
3	R	210	Total	C	H	N	O	S	0	0	0
			3195	1012	1583	272	323	5			
3	U	210	Total	C	H	N	O	S	0	0	0
			3193	1012	1581	272	323	5			
3	X	210	Total	C	H	N	O	S	0	0	0
			3198	1012	1586	272	323	5			

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

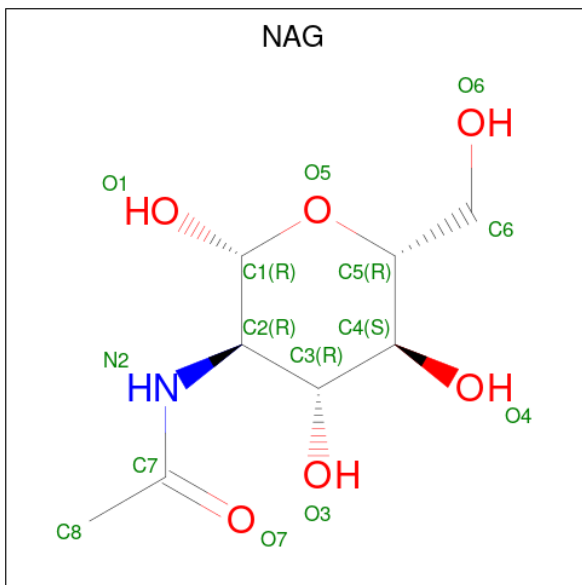
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
4	H	220	Total	C	H	N	O	S	0	0	0
			3322	1066	1648	283	320	5			
4	C	220	Total	C	H	N	O	S	0	0	0
			3245	1066	1571	283	320	5			
4	F	220	Total	C	H	N	O	S	0	0	0
			3186	1064	1515	283	319	5			
4	J	220	Total	C	H	N	O	S	0	0	0
			3186	1064	1515	283	319	5			
4	N	220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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

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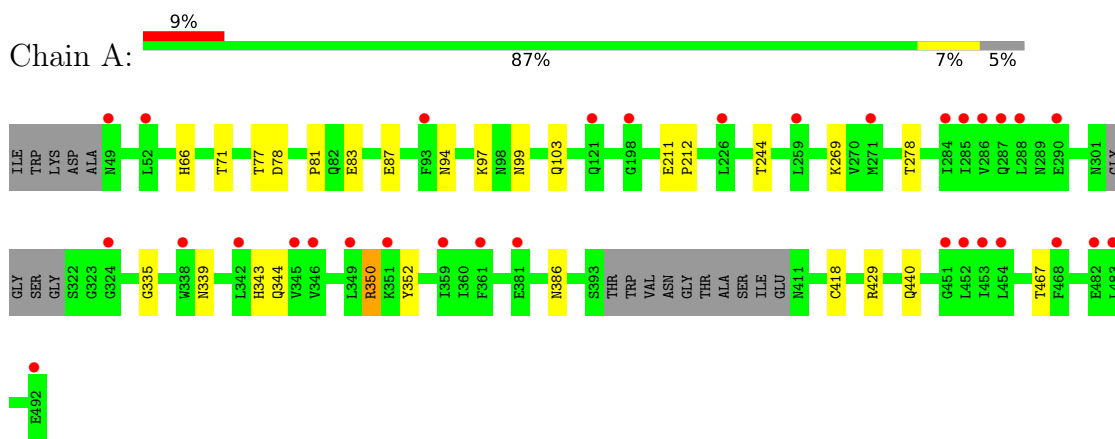
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>				<b>ZeroOcc</b>	<b>AltConf</b>
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	E	1	Total 14	C 8	N 1	O 5	0	0
5	M	1	Total 14	C 8	N 1	O 5	0	0
5	P	1	Total 14	C 8	N 1	O 5	0	0
5	P	1	Total 14	C 8	N 1	O 5	0	0
5	S	1	Total 14	C 8	N 1	O 5	0	0
5	S	1	Total 14	C 8	N 1	O 5	0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



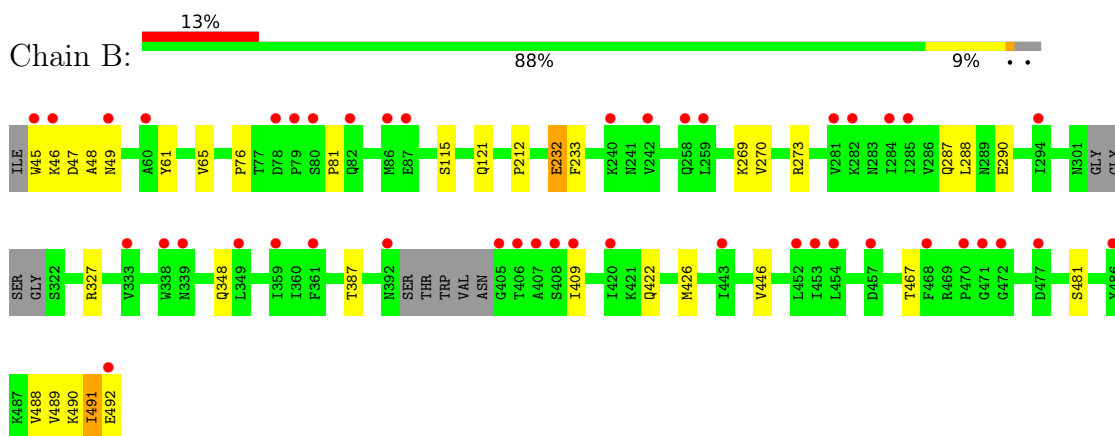
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

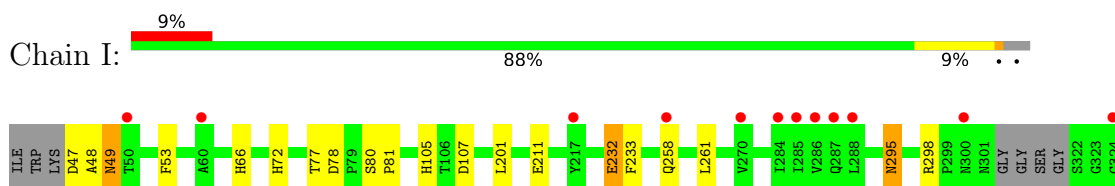
- Molecule 1: HIV-1 gp120

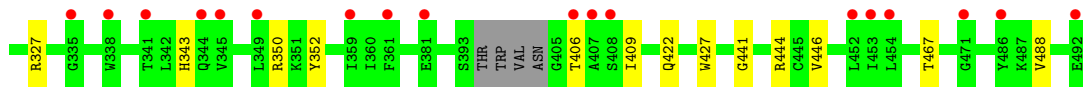


- Molecule 1: HIV-1 gp120

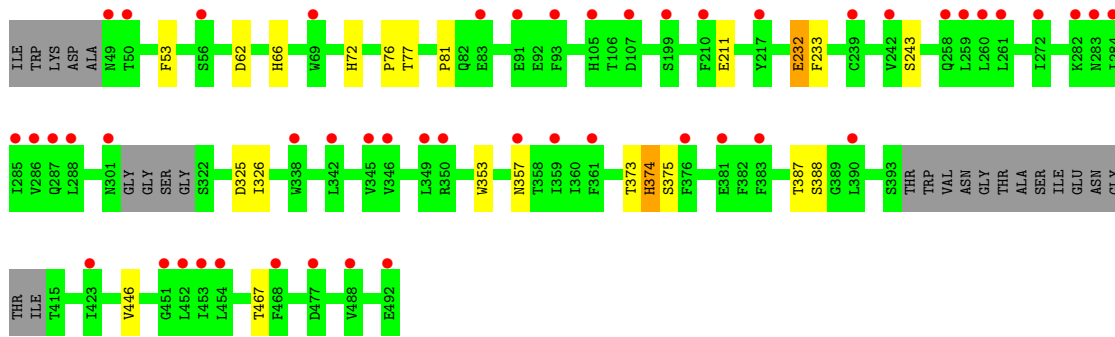
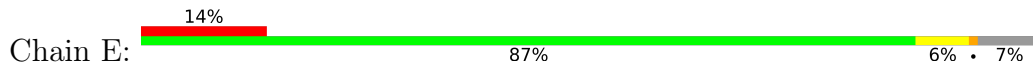


- Molecule 1: HIV-1 gp120

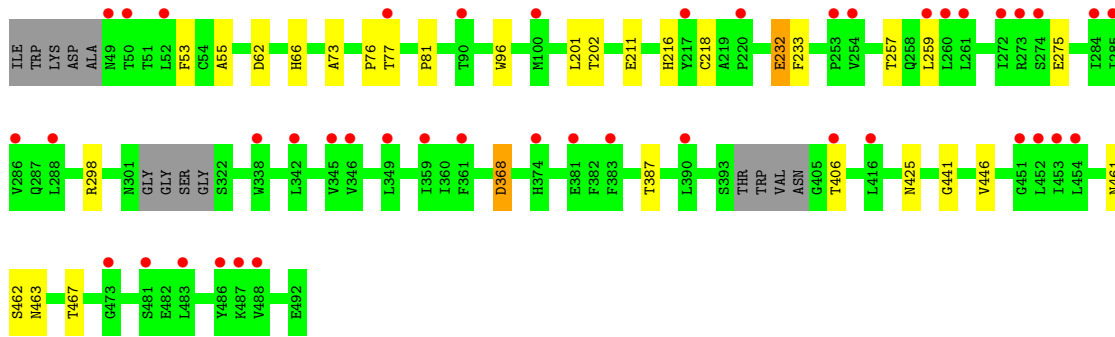
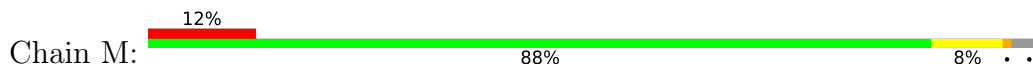




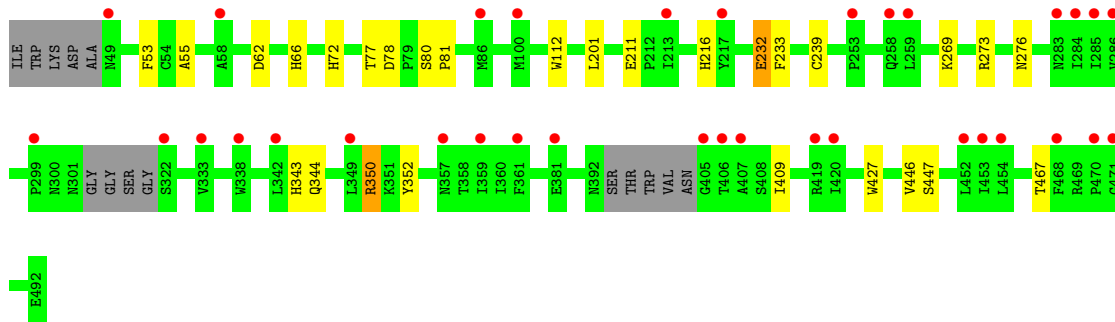
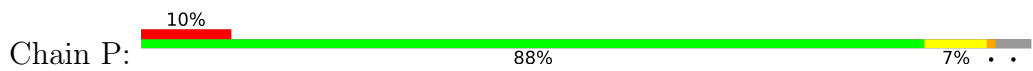
• Molecule 1: HIV-1 gp120



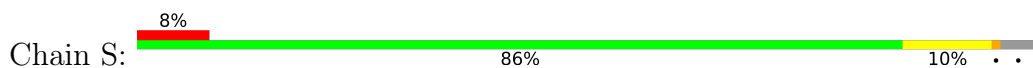
• Molecule 1: HIV-1 gp120

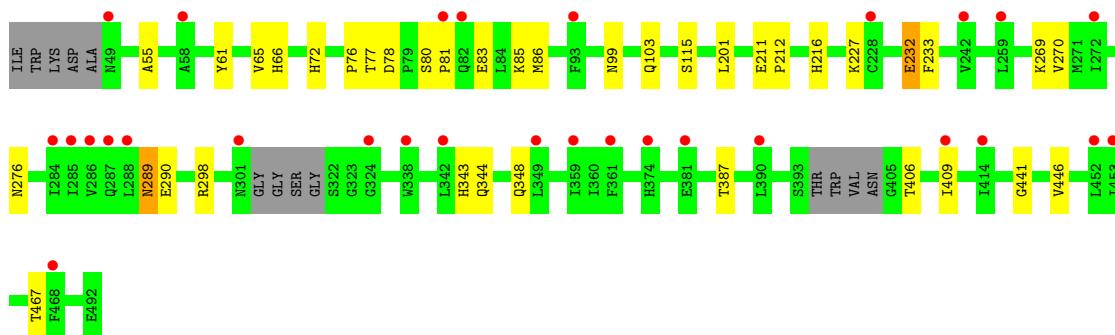


• Molecule 1: HIV-1 gp120

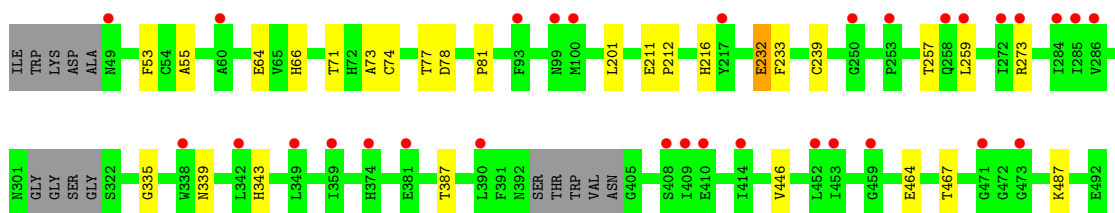
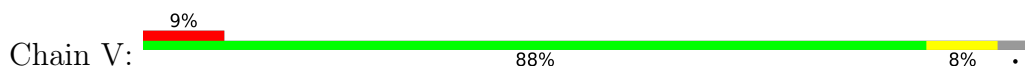


• Molecule 1: HIV-1 gp120

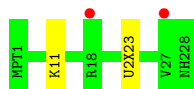
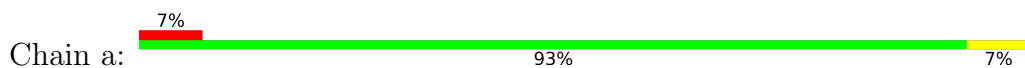




• Molecule 1: HIV-1 gp120



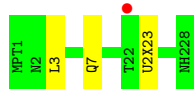
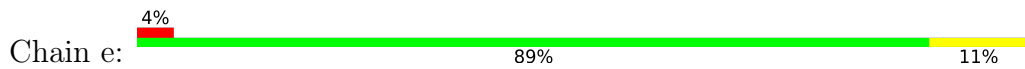
• Molecule 2: M48U1 peptide



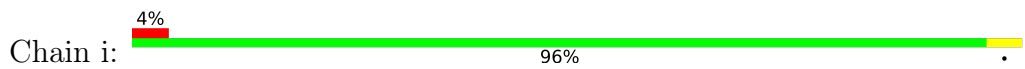
• Molecule 2: M48U1 peptide

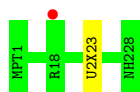


• Molecule 2: M48U1 peptide

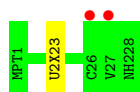


• Molecule 2: M48U1 peptide

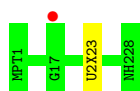
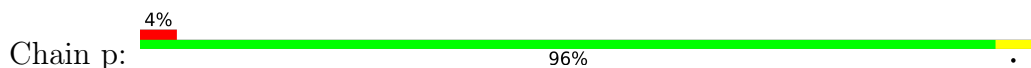




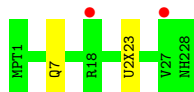
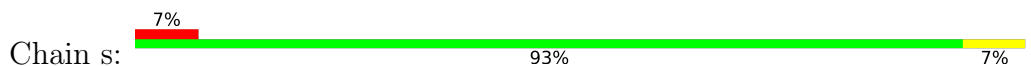
- Molecule 2: M48U1 peptide



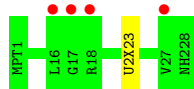
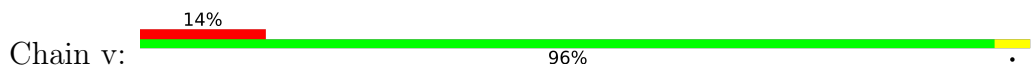
- Molecule 2: M48U1 peptide



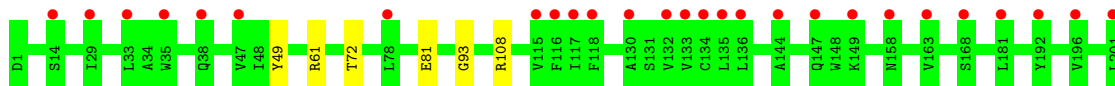
- Molecule 2: M48U1 peptide



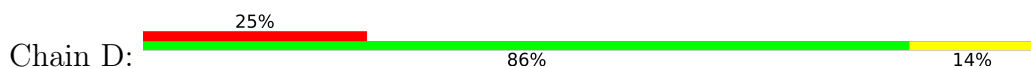
- Molecule 2: M48U1 peptide

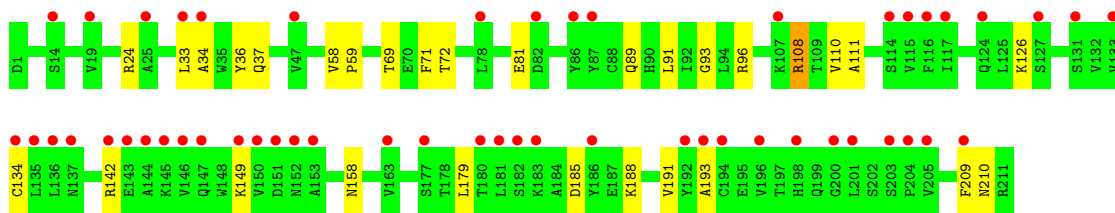


- Molecule 3: Antibody 2.2c LIGHT CHAIN

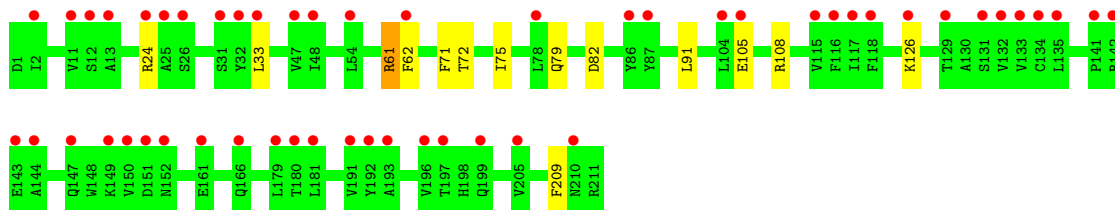


- Molecule 3: Antibody 2.2c LIGHT CHAIN

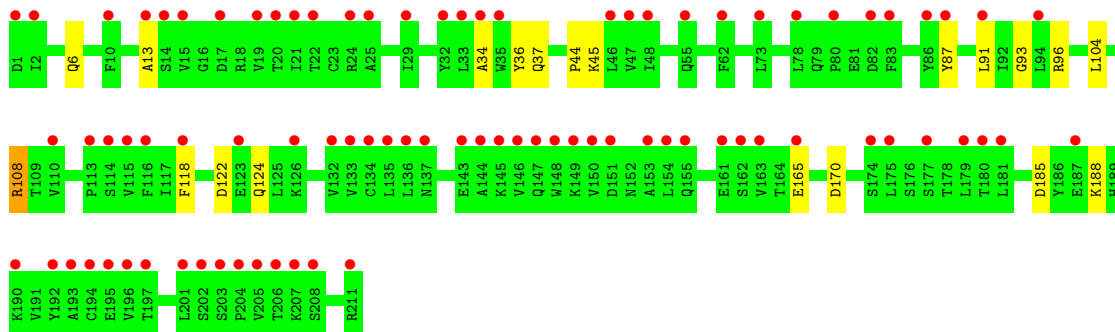
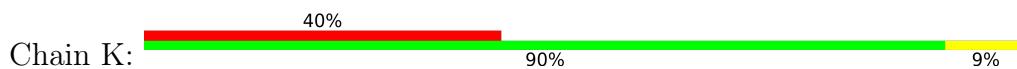




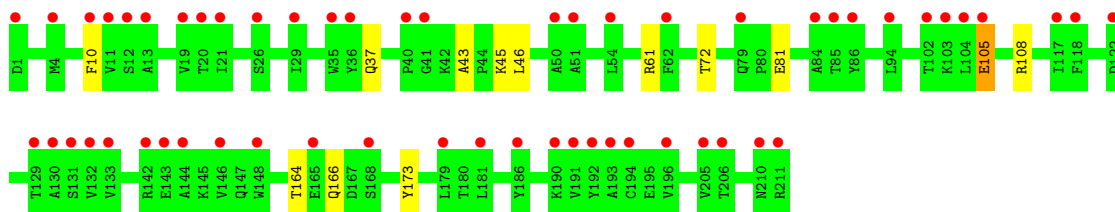
- Molecule 3: Antibody 2.2c LIGHT CHAIN



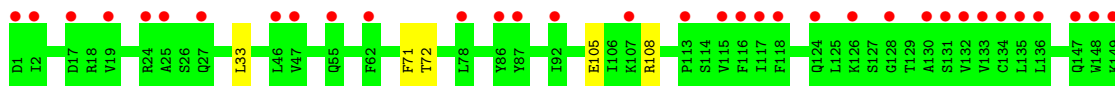
- Molecule 3: Antibody 2.2c LIGHT CHAIN

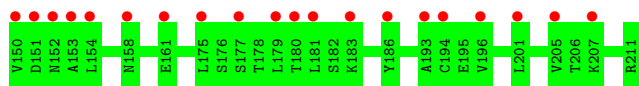


- Molecule 3: Antibody 2.2c LIGHT CHAIN

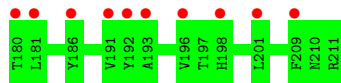


- Molecule 3: Antibody 2.2c LIGHT CHAIN

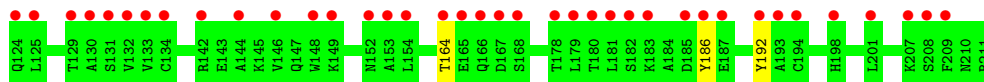
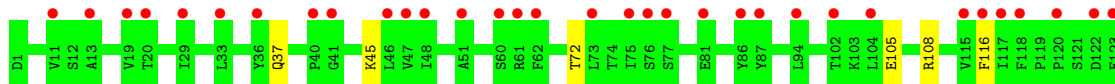




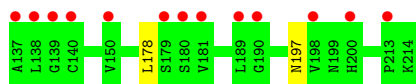
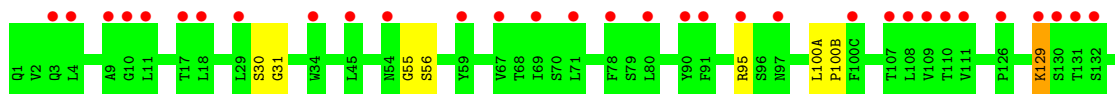
- Molecule 3: Antibody 2.2c LIGHT CHAIN



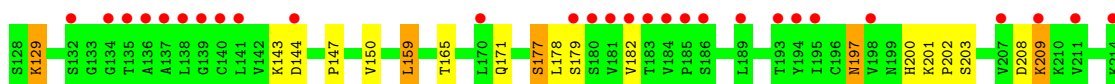
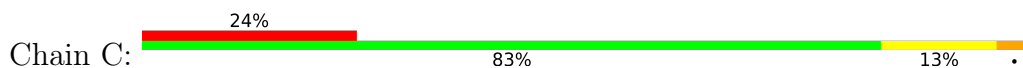
- Molecule 3: Antibody 2.2c LIGHT CHAIN



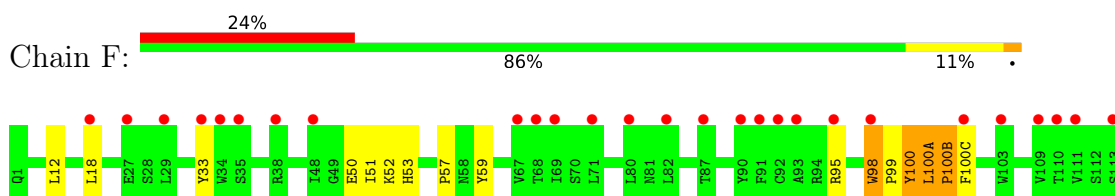
- Molecule 4: Antibody 2.2c heavy CHAIN



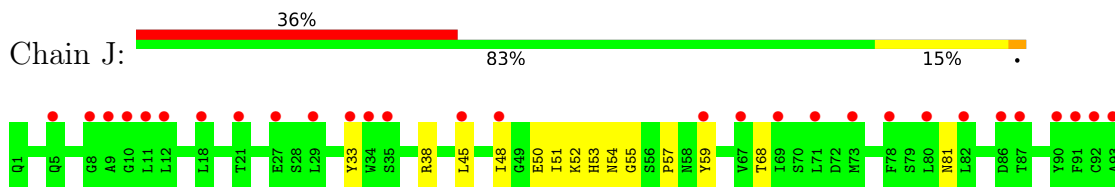
- Molecule 4: Antibody 2.2c heavy CHAIN



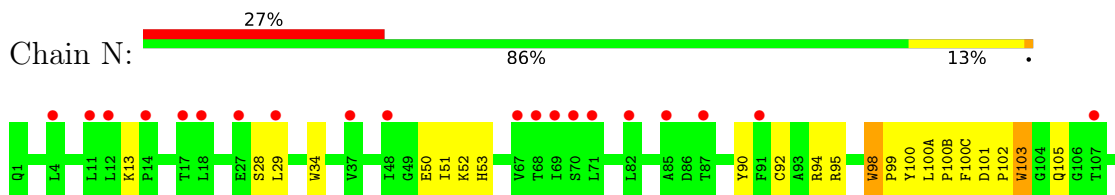
- Molecule 4: Antibody 2.2c heavy CHAIN



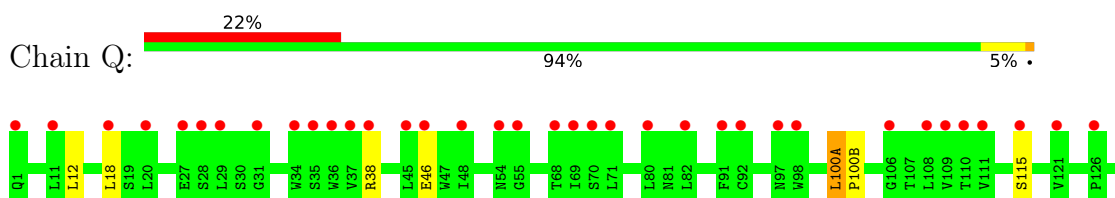
- Molecule 4: Antibody 2.2c heavy CHAIN



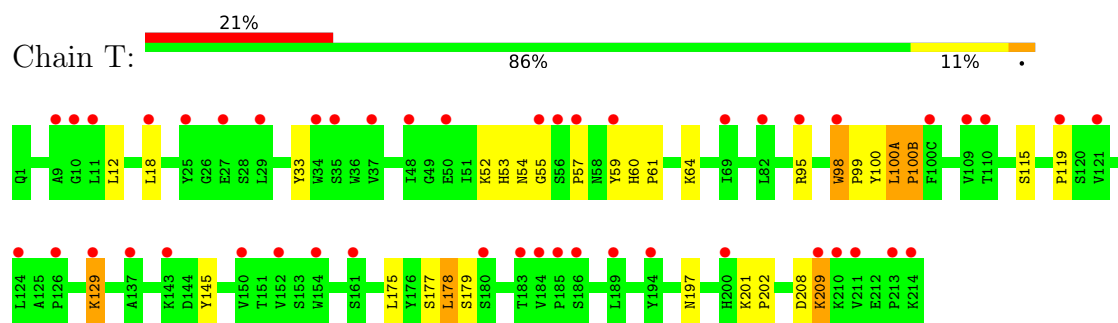
- Molecule 4: Antibody 2.2c heavy CHAIN



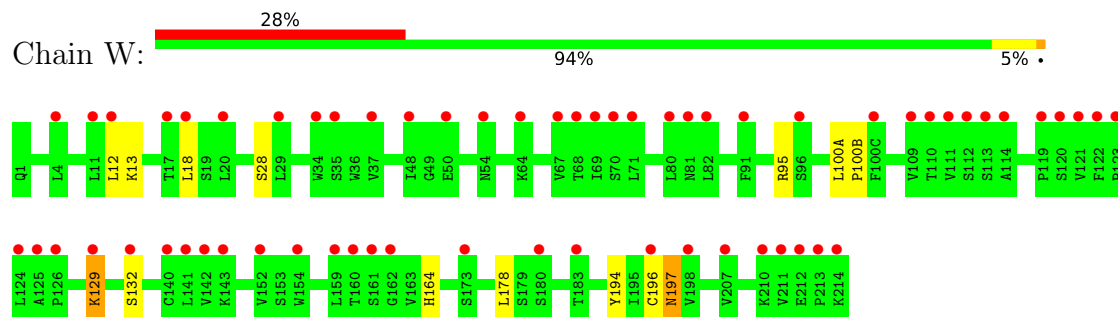
- Molecule 4: Antibody 2.2c heavy CHAIN



- Molecule 4: Antibody 2.2c heavy CHAIN



• 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, $\alpha$ , $\beta$ , $\gamma$	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) 33.3 (49.15-2.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.296 , 0.328 0.317 , 0.346	Depositor DCC
$R_{free}$ test set	3686 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.3	Xtrriage
Anisotropy	0.410	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 159.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality [i](#)

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

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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:O7	5:I:501:NAG:O3	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
3:G:91:LEU:CD2	4:F:100(B):PRO:HB3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:212:PRO:HG3	5:V:501:NAG:H2	1.74	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:446:VAL:O	5:B:501:NAG:H5	1.95	0.67
1:B:491:ILE:HG22	1:B:492:GLU:HG3	1.75	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:I:327:ARG:NH2	1:I:422:GLN:OE1	2.37	0.57
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: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:O7	5:B:502:NAG:O3	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
1:I:232:GLU:HB2	1:I:233:PHE:HA	1.91	0.53
4:F:98:TRP:HB3	4:F:100:TYR:HB2	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
5:I:501:NAG:H62	5:I:504:NAG:C8	2.41	0.50
4:F:95:ARG:HD3	4:F:100(C):PHE:CD1	2.47	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:N	1:A:87:GLU:OE1	2.45	0.49
3:X:37:GLN:O	3:X:45:LYS:N	2.46	0.49
3:X:186:TYR:O	3:X:192:TYR:OH	2.30	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
1:I:350:ARG:O	1:I:352:TYR:N	2.46	0.48
4:F:50:GLU:OE1	4:F:95:ARG:NH1	2.47	0.48
4:T:33:TYR:CZ	4:T:52:LYS:HD3	2.49	0.48
4:H:129:LYS:H	4:H:129:LYS:HD3	1.79	0.48
4:C:165:THR:O	4:C:165:THR:HG22	2.13	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)
3:O:164:THR:HG21	4:N:164:HIS:HB3	1.96	0.47
4:N:34:TRP:CH2	4:N:94:ARG:HG3	2.49	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:HD3	4:W:129:LYS:H	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
1:M:218:CYS:HB2	4:N:98:TRP:CZ2	2.51	0.46
4:N:34:TRP:CZ3	4:N:94:ARG:HB2	2.50	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
4:F:175:LEU:HD21	3:U:126:LYS:NZ	2.32	0.44
3:K:36:TYR:HH	4:J:100(B):PRO:HB2	1.83	0.44
4:Q:129:LYS:H	4:Q:129:LYS:HD3	1.82	0.44
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.53	0.44
4:C:200:HIS:CE1	4:C:202:PRO:HB2	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
3:G:61:ARG:CZ	3:G:79:GLN:NE2	2.81	0.44
4:F:95:ARG:HD3	4:F:100(C):PHE:CE1	2.53	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:I:295:ASN:HD22	1:I:444:ARG:NH2	2.15	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: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
1:B:61:TYR:HD2	4:C:61:PRO:HA	1.83	0.43
4:C:95:ARG:HB3	4:C:100(A):LEU:HD22	2.01	0.43
1:I:105:HIS:CE1	1:I:427:TRP:CZ2	3.06	0.43
4:H:100(A):LEU:N	4:H:100(B):PRO:HD2	2.34	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:H	4:T:129:LYS:HD3	1.82	0.43
1:A:71:THR:HG22	3:L:93:GLY:HA2	2.01	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: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:HB3	2.01	0.43
1:V:77:THR:HB	1:V:78:ASP:HA	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
4:F:203:SER:O	4:T:209:LYS:NZ	2.51	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:C:147:PRO:O	4:C:200:HIS:NE2	2.48	0.42
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.54	0.42
4:F:33:TYR:CZ	4:F:52:LYS:HD3	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:75:LYS:HG2	1:S:85:LYS:HD2	2.02	0.42
4:C:197:ASN:N	4:C:197:ASN:OD1	2.53	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:57:PRO:HB2	4:T:59:TYR:CE2	2.55	0.42
4:T:178:LEU:C	4:T:178:LEU:HD23	2.40	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
1:I:77:THR:HB	1:I:78:ASP:HB3	2.02	0.42
3:D:89:GLN:NE2	4:C:100(C):PHE:HE2	2.18	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
1:I:232:GLU:CB	1:I:233:PHE:CA	2.96	0.41
4:C:201:LYS:N	4:C:202:PRO:CD	2.84	0.41
1:M:201:LEU:HD23	1:M:202:THR:N	2.35	0.41
4:N:103:TRP:CD1	4:N:103:TRP:N	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
3:L:49:TYR:HB3	4:H:100(B):PRO:HG3	2.03	0.41
3:D:149:LYS:N	3:D:193:ALA:O	2.43	0.41
1:E:374:HIS:CD2	1:E:375:SER:N	2.89	0.41
3:G:62:PHE:CZ	3:G:75:ILE:HD13	2.56	0.41
3:G:209:PHE:HB3	4:F:129:LYS:NZ	2.35	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
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
4:C:127:SER:OG	4:C:129:LYS:CE	2.69	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:OE1	4:N:105:GLN:N	2.44	0.40
3:R:33:LEU:HD22	3:R:71:PHE:CG	2.57	0.40
1:I:48:ALA:HB3	1:I:488:VAL:HG12	2.03	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
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%)	17	57
1	B	336/352 (96%)	301 (90%)	29 (9%)	6 (2%)	8	43
1	E	323/352 (92%)	290 (90%)	26 (8%)	7 (2%)	6	39
1	I	335/352 (95%)	285 (85%)	42 (12%)	8 (2%)	6	37
1	M	333/352 (95%)	298 (90%)	28 (8%)	7 (2%)	7	40
1	P	332/352 (94%)	295 (89%)	30 (9%)	7 (2%)	7	40
1	S	333/352 (95%)	293 (88%)	34 (10%)	6 (2%)	8	43
1	V	332/352 (94%)	299 (90%)	29 (9%)	4 (1%)	13	52
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%)	29	67
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%)	11	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	8	43
4	H	217/220 (99%)	204 (94%)	13 (6%)	0	100	100
4	J	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	8	43
4	N	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	11	48
4	Q	217/220 (99%)	203 (94%)	13 (6%)	1 (0%)	29	67
4	T	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	11	48
4	W	217/220 (99%)	198 (91%)	18 (8%)	1 (0%)	29	67
All	All	6243/6480 (96%)	5748 (92%)	427 (7%)	68 (1%)	14	54

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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%)	55	79
1	B	299/306 (98%)	297 (99%)	2 (1%)	84	93
1	E	290/306 (95%)	288 (99%)	2 (1%)	84	93
1	I	298/306 (97%)	291 (98%)	7 (2%)	50	77
1	M	296/306 (97%)	293 (99%)	3 (1%)	76	89
1	P	295/306 (96%)	289 (98%)	6 (2%)	55	79
1	S	296/306 (97%)	290 (98%)	6 (2%)	55	79
1	V	296/306 (97%)	286 (97%)	10 (3%)	37	69
2	a	20/20 (100%)	19 (95%)	1 (5%)	24	59
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%)	33	66
3	G	183/183 (100%)	179 (98%)	4 (2%)	52	78
3	K	183/183 (100%)	182 (100%)	1 (0%)	88	95
3	L	183/183 (100%)	181 (99%)	2 (1%)	73	88
3	O	183/183 (100%)	180 (98%)	3 (2%)	62	83
3	R	183/183 (100%)	180 (98%)	3 (2%)	62	83
3	U	183/183 (100%)	178 (97%)	5 (3%)	44	74
3	X	183/183 (100%)	180 (98%)	3 (2%)	62	83
4	C	190/190 (100%)	180 (95%)	10 (5%)	22	58
4	F	190/190 (100%)	184 (97%)	6 (3%)	39	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	190/190 (100%)	186 (98%)	4 (2%)	53	79
4	J	190/190 (100%)	185 (97%)	5 (3%)	46	74
4	N	190/190 (100%)	179 (94%)	11 (6%)	20	55
4	Q	190/190 (100%)	187 (98%)	3 (2%)	62	83
4	T	190/190 (100%)	184 (97%)	6 (3%)	39	70
4	W	190/190 (100%)	183 (96%)	7 (4%)	34	67
All	All	5507/5592 (98%)	5384 (98%)	123 (2%)	52	78

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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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	J	30	4	4,5,9	0.85	0	0,5,11	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	OAS	F	30	4	4,5,9	0.85	0	0,5,11	-	-
2	U2X	b	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
2	U2X	p	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
2	U2X	m	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
4	OAS	W	30	4	7,8,9	0.81	0	5,9,11	0.68	0
2	U2X	i	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
4	OAS	N	30	4	4,5,9	0.80	0	0,5,11	-	-
4	OAS	H	30	4	7,8,9	0.78	0	5,9,11	0.84	0
2	U2X	s	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
4	OAS	Q	30	4	4,5,9	0.86	0	0,5,11	-	-
4	OAS	C	30	4	7,8,9	0.82	0	5,9,11	0.73	0
2	U2X	e	23	2	19,20,21	2.26	5 (26%)	22,25,27	1.79	7 (31%)
2	U2X	v	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)
4	OAS	T	30	4	7,8,9	0.81	0	5,9,11	0.76	0
2	U2X	a	23	2	19,20,21	2.27	5 (26%)	22,25,27	1.79	7 (31%)

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	J	30	4	-	0/2/4/9	-
4	OAS	F	30	4	-	0/2/4/9	-
2	U2X	b	23	2	-	5/10/19/21	0/2/2/2
2	U2X	p	23	2	-	5/10/19/21	0/2/2/2
2	U2X	m	23	2	-	5/10/19/21	0/2/2/2
4	OAS	W	30	4	-	2/5/7/9	-
2	U2X	i	23	2	-	5/10/19/21	0/2/2/2
4	OAS	N	30	4	-	0/2/4/9	-
4	OAS	H	30	4	-	5/5/7/9	-
2	U2X	s	23	2	-	5/10/19/21	0/2/2/2
4	OAS	Q	30	4	-	0/2/4/9	-
4	OAS	C	30	4	-	4/5/7/9	-
2	U2X	e	23	2	-	5/10/19/21	0/2/2/2
2	U2X	v	23	2	-	5/10/19/21	0/2/2/2
4	OAS	T	30	4	-	4/5/7/9	-
2	U2X	a	23	2	-	5/10/19/21	0/2/2/2

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	23	U2X	CE2-CD2	7.21	1.51	1.38
2	v	23	U2X	CE2-CD2	7.19	1.51	1.38
2	s	23	U2X	CE2-CD2	7.18	1.51	1.38
2	i	23	U2X	CE2-CD2	7.18	1.51	1.38
2	a	23	U2X	CE2-CD2	7.16	1.51	1.38
2	m	23	U2X	CE2-CD2	7.15	1.51	1.38
2	p	23	U2X	CE2-CD2	7.15	1.51	1.38
2	e	23	U2X	CE2-CD2	7.13	1.51	1.38
2	i	23	U2X	CE1-CD1	4.20	1.46	1.38
2	p	23	U2X	CE1-CD1	4.19	1.46	1.38
2	e	23	U2X	CE1-CD1	4.19	1.46	1.38
2	b	23	U2X	CE1-CD1	4.18	1.46	1.38
2	a	23	U2X	CE1-CD1	4.17	1.46	1.38
2	m	23	U2X	CE1-CD1	4.17	1.46	1.38
2	s	23	U2X	CE1-CD1	4.16	1.46	1.38
2	v	23	U2X	CE1-CD1	4.13	1.46	1.38
2	m	23	U2X	CE1-CZ	2.59	1.43	1.38
2	e	23	U2X	CE1-CZ	2.58	1.43	1.38
2	b	23	U2X	CE1-CZ	2.57	1.43	1.38
2	v	23	U2X	CE1-CZ	2.57	1.43	1.38
2	a	23	U2X	CE1-CZ	2.56	1.43	1.38
2	p	23	U2X	CE1-CZ	2.56	1.43	1.38
2	s	23	U2X	CE1-CZ	2.56	1.43	1.38
2	i	23	U2X	CE1-CZ	2.56	1.43	1.38
2	p	23	U2X	C4-C3	2.24	1.58	1.52
2	s	23	U2X	C4-C3	2.23	1.58	1.52
2	m	23	U2X	C4-C3	2.23	1.58	1.52
2	a	23	U2X	C4-C3	2.22	1.58	1.52
2	v	23	U2X	C4-C3	2.22	1.58	1.52
2	b	23	U2X	C4-C3	2.22	1.58	1.52
2	i	23	U2X	C4-C3	2.22	1.58	1.52
2	e	23	U2X	C4-C3	2.21	1.58	1.52
2	e	23	U2X	CB-CA	-2.04	1.49	1.53
2	p	23	U2X	CB-CA	-2.04	1.49	1.53
2	b	23	U2X	CB-CA	-2.04	1.49	1.53
2	a	23	U2X	CB-CA	-2.03	1.49	1.53
2	i	23	U2X	CB-CA	-2.02	1.49	1.53
2	m	23	U2X	CB-CA	-2.02	1.49	1.53
2	s	23	U2X	CB-CA	-2.02	1.49	1.53
2	v	23	U2X	CB-CA	-2.01	1.49	1.53

All (56) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	23	U2X	C2-C3-C7	4.13	121.66	111.28
2	e	23	U2X	C2-C3-C7	4.13	121.66	111.28
2	p	23	U2X	C2-C3-C7	4.13	121.65	111.28
2	i	23	U2X	C2-C3-C7	4.12	121.64	111.28
2	a	23	U2X	C2-C3-C7	4.12	121.63	111.28
2	v	23	U2X	C2-C3-C7	4.12	121.63	111.28
2	s	23	U2X	C2-C3-C7	4.12	121.63	111.28
2	b	23	U2X	C2-C3-C7	4.11	121.59	111.28
2	i	23	U2X	CG-CB-CA	2.95	120.07	114.10
2	e	23	U2X	CG-CB-CA	2.95	120.07	114.10
2	v	23	U2X	CG-CB-CA	2.95	120.07	114.10
2	b	23	U2X	CG-CB-CA	2.95	120.06	114.10
2	a	23	U2X	CG-CB-CA	2.94	120.05	114.10
2	m	23	U2X	CG-CB-CA	2.94	120.05	114.10
2	s	23	U2X	CG-CB-CA	2.93	120.03	114.10
2	p	23	U2X	CG-CB-CA	2.93	120.02	114.10
2	s	23	U2X	C4-C3-C7	2.82	118.37	111.28
2	i	23	U2X	C4-C3-C7	2.82	118.36	111.28
2	e	23	U2X	C4-C3-C7	2.81	118.35	111.28
2	b	23	U2X	C4-C3-C7	2.81	118.34	111.28
2	v	23	U2X	C4-C3-C7	2.81	118.34	111.28
2	m	23	U2X	C4-C3-C7	2.81	118.34	111.28
2	a	23	U2X	C4-C3-C7	2.81	118.33	111.28
2	p	23	U2X	C4-C3-C7	2.80	118.32	111.28
2	b	23	U2X	C1-C2-C3	-2.77	106.92	112.15
2	i	23	U2X	C1-C2-C3	-2.75	106.94	112.15
2	e	23	U2X	C1-C2-C3	-2.75	106.95	112.15
2	p	23	U2X	C1-C2-C3	-2.75	106.96	112.15
2	a	23	U2X	C1-C2-C3	-2.75	106.96	112.15
2	s	23	U2X	C1-C2-C3	-2.74	106.97	112.15
2	v	23	U2X	C1-C2-C3	-2.74	106.97	112.15
2	m	23	U2X	C1-C2-C3	-2.73	106.98	112.15
2	b	23	U2X	OH-C7-C3	2.34	114.31	108.21
2	p	23	U2X	OH-C7-C3	2.33	114.30	108.21
2	m	23	U2X	OH-C7-C3	2.33	114.29	108.21
2	a	23	U2X	OH-C7-C3	2.32	114.27	108.21
2	s	23	U2X	OH-C7-C3	2.32	114.26	108.21
2	i	23	U2X	OH-C7-C3	2.32	114.25	108.21
2	v	23	U2X	C5-C4-C3	-2.31	107.78	112.15
2	v	23	U2X	OH-C7-C3	2.31	114.25	108.21
2	e	23	U2X	OH-C7-C3	2.31	114.25	108.21
2	a	23	U2X	C5-C4-C3	-2.30	107.80	112.15
2	p	23	U2X	C5-C4-C3	-2.30	107.80	112.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	23	U2X	C5-C4-C3	-2.30	107.80	112.15
2	m	23	U2X	C5-C4-C3	-2.30	107.81	112.15
2	e	23	U2X	C5-C4-C3	-2.29	107.82	112.15
2	s	23	U2X	C5-C4-C3	-2.29	107.82	112.15
2	i	23	U2X	C5-C4-C3	-2.29	107.83	112.15
2	b	23	U2X	CD2-CG-CD1	2.21	121.64	118.17
2	s	23	U2X	CD2-CG-CD1	2.20	121.63	118.17
2	i	23	U2X	CD2-CG-CD1	2.20	121.62	118.17
2	p	23	U2X	CD2-CG-CD1	2.18	121.60	118.17
2	a	23	U2X	CD2-CG-CD1	2.18	121.59	118.17
2	m	23	U2X	CD2-CG-CD1	2.17	121.58	118.17
2	e	23	U2X	CD2-CG-CD1	2.17	121.58	118.17
2	v	23	U2X	CD2-CG-CD1	2.16	121.56	118.17

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	a	23	U2X	C2-C3-C7-OH
4	H	30	OAS	N-CA-CB-OG
4	H	30	OAS	C-CA-CB-OG
4	H	30	OAS	CA-CB-OG-C1A
2	b	23	U2X	C2-C3-C7-OH
4	C	30	OAS	C-CA-CB-OG
2	e	23	U2X	C2-C3-C7-OH
2	i	23	U2X	C2-C3-C7-OH
2	m	23	U2X	C2-C3-C7-OH
2	p	23	U2X	C2-C3-C7-OH
2	s	23	U2X	C2-C3-C7-OH
4	T	30	OAS	C-CA-CB-OG
2	v	23	U2X	C2-C3-C7-OH
4	H	30	OAS	C2A-C1A-OG-CB
4	T	30	OAS	C2A-C1A-OG-CB
4	H	30	OAS	OAC-C1A-OG-CB
4	T	30	OAS	OAC-C1A-OG-CB
4	W	30	OAS	OAC-C1A-OG-CB
4	W	30	OAS	C2A-C1A-OG-CB
4	C	30	OAS	C2A-C1A-OG-CB
4	C	30	OAS	OAC-C1A-OG-CB
2	a	23	U2X	C3-C7-OH-CZ
2	b	23	U2X	C3-C7-OH-CZ
2	e	23	U2X	C3-C7-OH-CZ

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Mol	Chain	Res	Type	Atoms
2	i	23	U2X	C3-C7-OH-CZ
2	m	23	U2X	C3-C7-OH-CZ
2	p	23	U2X	C3-C7-OH-CZ
2	s	23	U2X	C3-C7-OH-CZ
2	v	23	U2X	C3-C7-OH-CZ
4	C	30	OAS	N-CA-CB-OG
4	T	30	OAS	N-CA-CB-OG
2	b	23	U2X	CE2-CZ-OH-C7
2	p	23	U2X	CE2-CZ-OH-C7
2	a	23	U2X	CE2-CZ-OH-C7
2	e	23	U2X	CE2-CZ-OH-C7
2	i	23	U2X	CE2-CZ-OH-C7
2	m	23	U2X	CE2-CZ-OH-C7
2	s	23	U2X	CE2-CZ-OH-C7
2	v	23	U2X	CE2-CZ-OH-C7
2	e	23	U2X	CE1-CZ-OH-C7
2	m	23	U2X	CE1-CZ-OH-C7
2	p	23	U2X	CE1-CZ-OH-C7
2	s	23	U2X	CE1-CZ-OH-C7
2	v	23	U2X	CE1-CZ-OH-C7
2	a	23	U2X	CE1-CZ-OH-C7
2	b	23	U2X	CE1-CZ-OH-C7
2	i	23	U2X	CE1-CZ-OH-C7
2	a	23	U2X	C4-C3-C7-OH
2	b	23	U2X	C4-C3-C7-OH
2	e	23	U2X	C4-C3-C7-OH
2	i	23	U2X	C4-C3-C7-OH
2	m	23	U2X	C4-C3-C7-OH
2	p	23	U2X	C4-C3-C7-OH
2	s	23	U2X	C4-C3-C7-OH
2	v	23	U2X	C4-C3-C7-OH

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 monosaccharides in this entry.

## 5.6 Ligand geometry

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	M	501	1	14,14,15	0.27	0	17,19,21	0.45	0
5	NAG	A	503	1	14,14,15	0.21	0	17,19,21	0.43	0
5	NAG	B	502	1	14,14,15	0.35	0	17,19,21	1.27	1 (5%)
5	NAG	A	501	1	14,14,15	0.45	0	17,19,21	0.39	0
5	NAG	A	504	1	14,14,15	0.19	0	17,19,21	0.39	0
5	NAG	I	504	1	14,14,15	0.52	0	17,19,21	0.35	0
5	NAG	I	502	1	14,14,15	0.35	0	17,19,21	0.45	0
5	NAG	S	502	1	14,14,15	0.48	0	17,19,21	0.79	1 (5%)
5	NAG	P	502	1	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	E	502	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	E	501	1	14,14,15	0.28	0	17,19,21	0.39	0
5	NAG	B	501	1	14,14,15	0.23	0	17,19,21	0.41	0
5	NAG	V	501	1	14,14,15	0.34	0	17,19,21	0.39	0
5	NAG	S	501	1	14,14,15	0.24	0	17,19,21	0.39	0
5	NAG	P	501	1	14,14,15	0.23	0	17,19,21	0.35	0
5	NAG	I	503	1	14,14,15	0.22	0	17,19,21	0.41	0
5	NAG	S	503	1	14,14,15	0.28	0	17,19,21	0.37	0
5	NAG	I	501	1	14,14,15	0.28	0	17,19,21	0.49	0
5	NAG	A	502	1	14,14,15	0.27	0	17,19,21	0.41	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	M	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	503	1	-	4/6/23/26	0/1/1/1
5	NAG	B	502	1	-	4/6/23/26	0/1/1/1
5	NAG	A	501	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	504	1	-	2/6/23/26	0/1/1/1
5	NAG	I	504	1	-	4/6/23/26	0/1/1/1
5	NAG	I	502	1	-	4/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	P	502	1	-	1/6/23/26	0/1/1/1
5	NAG	E	502	1	-	0/6/23/26	0/1/1/1
5	NAG	E	501	1	-	2/6/23/26	0/1/1/1
5	NAG	B	501	1	-	2/6/23/26	0/1/1/1
5	NAG	V	501	1	-	4/6/23/26	0/1/1/1
5	NAG	S	501	1	-	2/6/23/26	0/1/1/1
5	NAG	P	501	1	-	2/6/23/26	0/1/1/1
5	NAG	I	503	1	-	4/6/23/26	0/1/1/1
5	NAG	S	503	1	-	4/6/23/26	0/1/1/1
5	NAG	I	501	1	-	2/6/23/26	0/1/1/1
5	NAG	A	502	1	-	2/6/23/26	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	B	502	NAG	C1-O5-C5	4.30	118.01	112.19
5	S	502	NAG	C1-C2-N2	2.17	114.20	110.49

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	501	NAG	O5-C5-C6-O6
5	S	501	NAG	O5-C5-C6-O6
5	A	503	NAG	C4-C5-C6-O6
5	I	504	NAG	O5-C5-C6-O6
5	B	501	NAG	O5-C5-C6-O6
5	I	503	NAG	O5-C5-C6-O6
5	E	501	NAG	O5-C5-C6-O6
5	B	502	NAG	O5-C5-C6-O6
5	B	501	NAG	C4-C5-C6-O6
5	P	501	NAG	C4-C5-C6-O6
5	A	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	503	NAG	O5-C5-C6-O6
5	I	504	NAG	C4-C5-C6-O6
5	S	501	NAG	C4-C5-C6-O6
5	I	504	NAG	C1-C2-N2-C7
5	A	502	NAG	O5-C5-C6-O6
5	A	501	NAG	C4-C5-C6-O6
5	A	503	NAG	C8-C7-N2-C2
5	A	503	NAG	O7-C7-N2-C2
5	A	504	NAG	C8-C7-N2-C2
5	A	504	NAG	O7-C7-N2-C2
5	I	503	NAG	C8-C7-N2-C2
5	I	503	NAG	O7-C7-N2-C2
5	S	503	NAG	C8-C7-N2-C2
5	S	503	NAG	O7-C7-N2-C2
5	I	503	NAG	C4-C5-C6-O6
5	I	502	NAG	O5-C5-C6-O6
5	A	502	NAG	C4-C5-C6-O6
5	E	501	NAG	C4-C5-C6-O6
5	B	502	NAG	C1-C2-N2-C7
5	S	503	NAG	O5-C5-C6-O6
5	S	503	NAG	C4-C5-C6-O6
5	I	502	NAG	C1-C2-N2-C7
5	M	501	NAG	O5-C5-C6-O6
5	M	501	NAG	C4-C5-C6-O6
5	I	501	NAG	C1-C2-N2-C7
5	I	502	NAG	C4-C5-C6-O6
5	V	501	NAG	C1-C2-N2-C7
5	B	502	NAG	C4-C5-C6-O6
5	I	501	NAG	C3-C2-N2-C7
5	P	502	NAG	O5-C5-C6-O6
5	V	501	NAG	C4-C5-C6-O6
5	I	502	NAG	C3-C2-N2-C7
5	B	502	NAG	C3-C2-N2-C7
5	I	504	NAG	C3-C2-N2-C7
5	V	501	NAG	C3-C2-N2-C7
5	V	501	NAG	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	501	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	503	NAG	1	0
5	B	502	NAG	7	0
5	A	501	NAG	2	0
5	A	504	NAG	2	0
5	I	504	NAG	3	0
5	S	502	NAG	11	0
5	P	502	NAG	3	0
5	E	502	NAG	1	0
5	E	501	NAG	1	0
5	B	501	NAG	3	0
5	V	501	NAG	3	0
5	S	501	NAG	2	0
5	P	501	NAG	2	0
5	I	501	NAG	6	0
5	A	502	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	333/352 (94%)	0.56	32 (9%) 8 5	119, 153, 203, 222	0
1	B	342/352 (97%)	0.61	44 (12%) 3 3	105, 174, 268, 299	0
1	E	329/352 (93%)	0.71	49 (14%) 2 2	141, 205, 256, 283	0
1	I	341/352 (96%)	0.41	30 (8%) 10 6	120, 166, 210, 232	0
1	M	339/352 (96%)	0.60	43 (12%) 3 3	122, 188, 245, 262	0
1	P	338/352 (96%)	0.56	34 (10%) 7 4	104, 170, 241, 263	0
1	S	339/352 (96%)	0.56	29 (8%) 10 7	123, 177, 252, 283	0
1	V	338/352 (96%)	0.59	31 (9%) 9 5	122, 180, 263, 301	0
2	a	24/28 (85%)	0.38	2 (8%) 11 8	141, 188, 204, 208	0
2	b	24/28 (85%)	0.30	1 (4%) 36 23	161, 195, 225, 229	0
2	e	24/28 (85%)	0.16	1 (4%) 36 23	171, 198, 220, 223	0
2	i	24/28 (85%)	0.13	1 (4%) 36 23	140, 189, 200, 204	0
2	m	24/28 (85%)	0.38	2 (8%) 11 8	171, 209, 228, 233	0
2	p	24/28 (85%)	0.36	1 (4%) 36 23	118, 160, 181, 188	0
2	s	24/28 (85%)	0.37	2 (8%) 11 8	149, 202, 226, 231	0
2	v	24/28 (85%)	0.36	4 (16%) 1 1	170, 213, 220, 221	0
3	D	210/210 (100%)	1.35	52 (24%) 0 0	106, 227, 332, 347	0
3	G	210/210 (100%)	1.39	52 (24%) 0 0	172, 252, 328, 358	0
3	K	210/210 (100%)	2.85	85 (40%) 0 0	210, 340, 366, 371	0
3	L	210/210 (100%)	0.61	28 (13%) 3 3	146, 230, 276, 302	0
3	O	210/210 (100%)	1.26	56 (26%) 0 0	193, 256, 292, 314	0
3	R	210/210 (100%)	1.35	54 (25%) 0 0	181, 250, 340, 377	0
3	U	210/210 (100%)	0.75	34 (16%) 1 1	117, 227, 317, 334	0
3	X	210/210 (100%)	1.49	71 (33%) 0 0	185, 248, 303, 317	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9	
4	C	219/220 (99%)	1.08	52 (23%)	0	0	102, 188, 337, 353	0
4	F	219/220 (99%)	1.02	52 (23%)	0	0	189, 240, 283, 314	0
4	H	219/220 (99%)	0.70	45 (20%)	1	0	144, 198, 268, 280	0
4	J	219/220 (99%)	1.89	79 (36%)	0	0	205, 303, 380, 398	0
4	N	219/220 (99%)	1.39	59 (26%)	0	0	189, 240, 282, 300	0
4	Q	219/220 (99%)	0.92	49 (22%)	0	0	179, 241, 285, 310	0
4	T	219/220 (99%)	1.12	47 (21%)	0	0	125, 212, 311, 338	0
4	W	219/220 (99%)	1.19	62 (28%)	0	0	170, 232, 271, 292	0
All	All	6323/6480 (97%)	0.95	1183 (18%)	1	0	102, 208, 323, 398	0

All (1183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	197	THR	29.6
3	K	136	LEU	28.1
4	J	179	SER	24.5
3	K	144	ALA	24.5
3	K	115	VAL	23.1
3	D	193	ALA	18.9
3	R	149	LYS	18.0
4	J	11	LEU	16.8
3	K	175	LEU	16.5
3	K	34	ALA	16.2
3	G	150	VAL	15.0
3	K	145	LYS	14.8
3	U	181	LEU	14.3
4	T	211	VAL	13.8
4	J	109	VAL	13.7
3	R	150	VAL	13.5
4	N	184	VAL	13.2
3	G	181	LEU	13.1
3	K	177	SER	13.0
3	K	21	ILE	13.0
4	F	179	SER	12.9
1	V	459	GLY	12.9
3	D	209	PHE	12.9
3	K	19	VAL	12.8
1	P	406	THR	12.8
3	K	73	LEU	12.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	C	180	SER	12.5
4	T	161	SER	12.4
3	G	132	VAL	12.3
4	J	147	PRO	12.3
3	K	135	LEU	12.1
4	F	69	ILE	12.1
1	E	453	ILE	12.0
1	M	285	ILE	11.7
1	A	359	ILE	11.3
3	D	181	LEU	10.8
3	O	11	VAL	10.7
3	D	150	VAL	10.6
3	X	132	VAL	10.6
3	K	116	PHE	10.5
3	O	104	LEU	10.3
3	G	149	LYS	10.1
4	T	126	PRO	10.0
3	K	161	GLU	10.0
4	J	12	LEU	10.0
3	G	192	TYR	9.8
4	W	211	VAL	9.7
3	D	135	LEU	9.7
3	G	131	SER	9.6
3	G	116	PHE	9.6
3	G	25	ALA	9.6
4	W	119	PRO	9.5
1	V	359	ILE	9.5
4	N	129	LYS	9.5
3	K	134	CYS	9.5
3	O	192	TYR	9.4
3	K	20	THR	9.4
4	N	114	ALA	9.4
1	M	359	ILE	9.3
1	S	359	ILE	9.3
3	G	133	VAL	9.3
3	X	186	TYR	9.2
1	B	408	SER	9.2
4	F	180	SER	9.2
4	F	129	LYS	9.0
3	K	204	PRO	9.0
3	O	131	SER	9.0
4	C	211	VAL	8.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	R	116	PHE	8.9
3	O	51	ALA	8.9
4	J	178	LEU	8.8
1	E	286	VAL	8.8
3	X	131	SER	8.7
3	D	134	CYS	8.7
1	M	286	VAL	8.7
4	Q	111	VAL	8.7
3	K	14	SER	8.6
3	L	181	LEU	8.6
1	E	452	LEU	8.6
3	D	192	TYR	8.5
4	Q	140	CYS	8.5
4	C	184	VAL	8.5
4	J	69	ILE	8.4
4	N	112	SER	8.4
3	D	144	ALA	8.4
1	E	284	ILE	8.2
3	G	47	VAL	8.2
4	W	69	ILE	8.1
1	E	283	ASN	8.1
3	R	181	LEU	7.9
4	W	112	SER	7.9
3	R	133	VAL	7.9
3	K	203	SER	7.8
3	D	149	LYS	7.8
3	X	117	ILE	7.8
3	X	133	VAL	7.8
1	E	285	ILE	7.7
4	J	9	ALA	7.7
3	X	193	ALA	7.6
1	S	338	TRP	7.6
1	P	453	ILE	7.6
3	R	134	CYS	7.5
3	K	196	VAL	7.5
3	R	193	ALA	7.5
4	J	180	SER	7.5
4	N	179	SER	7.4
3	D	152	ASN	7.4
4	N	18	LEU	7.4
4	W	29	LEU	7.3
3	K	33	LEU	7.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	191	VAL	7.3
3	O	50	ALA	7.3
3	K	82	ASP	7.3
3	X	194	CYS	7.2
3	U	17	ASP	7.2
1	S	286	VAL	7.2
4	C	140	CYS	7.2
4	C	138	LEU	7.2
3	K	180	THR	7.2
4	N	130	SER	7.2
4	C	185	PRO	7.2
3	K	133	VAL	7.1
3	R	180	THR	7.1
3	X	62	PHE	7.1
4	F	111	VAL	7.1
4	J	33	TYR	7.1
1	E	258	GLN	7.1
3	X	207	LYS	7.0
3	U	209	PHE	7.0
4	W	18	LEU	7.0
4	J	110	THR	7.0
4	N	111	VAL	6.9
3	X	181	LEU	6.9
4	H	54	ASN	6.9
3	G	193	ALA	6.9
3	R	86	TYR	6.8
1	P	284	ILE	6.8
3	O	142	ARG	6.8
4	J	194	TYR	6.8
4	N	82	LEU	6.8
3	K	46	LEU	6.7
3	D	205	VAL	6.7
1	B	453	ILE	6.7
3	K	147	GLN	6.7
4	F	141	LEU	6.7
4	N	160	THR	6.7
3	R	201	LEU	6.7
4	W	67	VAL	6.7
4	J	18	LEU	6.7
4	J	35	SER	6.6
4	F	48	ILE	6.6
4	F	181	VAL	6.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	C	183	THR	6.6
3	K	113	PRO	6.6
3	K	47	VAL	6.6
3	G	12	SER	6.6
4	Q	38	ARG	6.6
4	Q	29	LEU	6.6
1	A	284	ILE	6.5
4	F	93	ALA	6.5
4	F	29	LEU	6.5
1	A	286	VAL	6.5
1	M	259	LEU	6.5
3	K	13	ALA	6.5
3	D	25	ALA	6.4
3	K	205	VAL	6.4
1	E	454	LEU	6.4
4	J	123	PRO	6.4
4	C	139	GLY	6.4
1	A	452	LEU	6.3
3	K	181	LEU	6.3
3	U	113	PRO	6.3
4	F	142	VAL	6.3
1	M	452	LEU	6.3
3	O	12	SER	6.3
4	W	126	PRO	6.3
4	W	160	THR	6.3
4	Q	179	SER	6.3
4	C	181	VAL	6.3
1	V	338	TRP	6.3
3	G	87	TYR	6.2
3	K	25	ALA	6.2
3	K	154	LEU	6.2
3	O	54	LEU	6.2
4	Q	27	GLU	6.2
1	M	284	ILE	6.2
4	J	130	SER	6.1
3	G	32	TYR	6.1
4	J	129	LYS	6.1
1	P	452	LEU	6.1
3	G	151	ASP	6.1
4	H	189	LEU	6.1
4	J	164	HIS	6.1
1	M	473	GLY	6.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	X	76	SER	6.1
1	S	259	LEU	6.0
1	E	349	LEU	6.0
4	J	166	PHE	6.0
4	J	137	ALA	6.0
3	X	29	ILE	6.0
1	I	286	VAL	6.0
4	F	67	VAL	6.0
3	R	135	LEU	6.0
1	V	93	PHE	5.9
3	K	146	VAL	5.9
4	T	110	THR	5.9
1	M	349	LEU	5.9
3	L	192	TYR	5.9
4	Q	37	VAL	5.9
3	O	4	MET	5.9
4	N	110	THR	5.9
3	D	201	LEU	5.9
3	O	29	ILE	5.9
3	U	151	ASP	5.9
3	X	41	GLY	5.9
4	C	18	LEU	5.9
4	W	121	VAL	5.9
3	L	116	PHE	5.9
3	K	174	SER	5.9
4	C	11	LEU	5.9
4	N	126	PRO	5.9
3	G	11	VAL	5.9
1	V	452	LEU	5.9
3	G	13	ALA	5.8
3	L	115	VAL	5.8
1	B	359	ILE	5.8
1	S	414	ILE	5.8
3	R	205	VAL	5.8
3	O	86	TYR	5.8
3	X	36	TYR	5.8
4	C	35	SER	5.8
4	H	138	LEU	5.7
3	R	25	ALA	5.7
3	X	168	SER	5.7
3	K	87	TYR	5.7
3	G	118	PHE	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	K	165	GLU	5.7
1	B	259	LEU	5.7
4	C	194	TYR	5.7
3	D	131	SER	5.7
2	a	27	VAL	5.6
4	W	37	VAL	5.6
1	M	338	TRP	5.6
3	G	196	VAL	5.6
4	J	34	TRP	5.6
3	X	192	TYR	5.6
3	R	196	VAL	5.6
1	B	338	TRP	5.6
4	J	71	LEU	5.6
4	Q	35	SER	5.5
3	X	148	TRP	5.5
1	A	290	GLU	5.5
3	K	155	GLN	5.5
4	H	150	VAL	5.5
4	J	59	TYR	5.5
3	L	133	VAL	5.4
4	N	136	ALA	5.4
1	B	242	VAL	5.4
1	P	359	ILE	5.4
3	O	132	VAL	5.4
4	T	109	VAL	5.4
1	V	259	LEU	5.4
4	T	29	LEU	5.4
1	V	409	ILE	5.4
4	H	90	TYR	5.4
3	K	15	VAL	5.3
4	W	111	VAL	5.3
4	T	186	SER	5.3
4	J	149	PRO	5.3
3	D	180	THR	5.3
3	K	150	VAL	5.3
1	I	407	ALA	5.2
4	N	107	THR	5.2
3	G	86	TYR	5.2
1	I	287	GLN	5.2
4	T	9	ALA	5.2
1	M	361	PHE	5.2
4	F	150	VAL	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	258	GLN	5.2
3	D	147	GLN	5.2
3	D	198	HIS	5.2
4	N	69	ILE	5.2
4	W	110	THR	5.2
4	H	11	LEU	5.2
4	N	198	VAL	5.1
4	C	123	PRO	5.1
4	C	82	LEU	5.1
4	J	165	THR	5.1
1	A	453	ILE	5.1
3	K	206	THR	5.1
4	J	210	LYS	5.1
1	A	285	ILE	5.1
1	I	359	ILE	5.1
3	L	35	TRP	5.1
1	V	253	PRO	5.1
3	D	136	LEU	5.0
1	M	488	VAL	5.0
1	E	359	ILE	5.0
3	R	207	LYS	5.0
3	K	211	ARG	5.0
4	W	96	SER	5.0
1	M	50	THR	5.0
4	T	18	LEU	5.0
3	K	114	SER	5.0
3	O	41	GLY	5.0
4	W	132	SER	5.0
4	W	161	SER	5.0
3	L	135	LEU	5.0
1	V	453	ILE	5.0
1	B	407	ALA	4.9
1	M	77	THR	4.9
4	C	122	PHE	4.9
3	K	194	CYS	4.9
4	F	109	VAL	4.9
4	J	87	THR	4.9
3	D	153	ALA	4.9
4	H	110	THR	4.9
1	I	285	ILE	4.9
2	p	17	GLY	4.9
4	N	71	LEU	4.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	T	129	LYS	4.9
3	U	193	ALA	4.9
4	T	209	LYS	4.9
3	R	47	VAL	4.9
3	R	24	ARG	4.8
1	P	454	LEU	4.8
4	H	10	GLY	4.8
3	K	62	PHE	4.8
1	V	272	ILE	4.8
4	J	108	LEU	4.8
4	J	195	ILE	4.7
3	D	196	VAL	4.7
4	H	109	VAL	4.7
4	T	25	TYR	4.7
4	C	108	LEU	4.7
3	R	132	VAL	4.7
4	F	35	SER	4.7
3	O	130	ALA	4.7
3	R	87	TYR	4.7
4	Q	36	TRP	4.7
1	B	281	VAL	4.7
4	T	34	TRP	4.7
4	J	8	GLY	4.7
3	G	33	LEU	4.7
1	P	338	TRP	4.7
4	W	82	LEU	4.7
4	T	82	LEU	4.6
3	R	19	VAL	4.6
4	J	148	GLU	4.6
3	U	142	ARG	4.6
4	W	71	LEU	4.6
1	V	284	ILE	4.6
3	O	103	LYS	4.6
3	R	62	PHE	4.6
1	M	260	LEU	4.6
4	N	185	PRO	4.6
4	C	186	SER	4.6
4	J	29	LEU	4.6
3	O	210	ASN	4.6
1	V	258	GLN	4.6
3	G	117	ILE	4.6
3	R	151	ASP	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	T	214	LYS	4.6
1	P	471	GLY	4.5
4	W	213	PRO	4.5
3	D	115	VAL	4.5
3	O	144	ALA	4.5
4	J	27	GLU	4.5
1	A	287	GLN	4.5
4	N	11	LEU	4.5
3	X	51	ALA	4.5
1	A	492	GLU	4.5
3	G	161	GLU	4.4
4	J	86	ASP	4.4
1	M	254	VAL	4.4
3	K	149	LYS	4.4
3	L	78	LEU	4.4
3	U	150	VAL	4.4
3	O	118	PHE	4.4
3	O	62	PHE	4.4
4	T	56	SER	4.4
1	V	473	GLY	4.4
4	Q	110	THR	4.4
1	E	357	ASN	4.4
4	F	100(C)	PHE	4.3
4	W	207	VAL	4.3
1	V	390	LEU	4.3
4	H	17	THR	4.3
4	Q	80	LEU	4.3
2	s	27	VAL	4.3
3	R	152	ASN	4.3
1	A	483	LEU	4.3
3	D	86	TYR	4.3
3	U	192	TYR	4.3
1	I	50	THR	4.3
4	H	108	LEU	4.3
1	E	259	LEU	4.3
4	H	18	LEU	4.3
3	R	128	GLY	4.3
1	S	285	ILE	4.3
4	F	27	GLU	4.3
1	B	452	LEU	4.3
3	G	24	ARG	4.2
4	W	12	LEU	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	47	VAL	4.2
4	H	80	LEU	4.2
1	E	242	VAL	4.2
3	X	129	THR	4.2
3	L	144	ALA	4.2
4	Q	69	ILE	4.2
1	B	86	MET	4.2
3	G	135	LEU	4.2
3	O	10	PHE	4.2
1	A	451	GLY	4.1
4	H	213	PRO	4.1
4	T	10	GLY	4.1
3	L	134	CYS	4.1
1	P	258	GLN	4.1
4	C	126	PRO	4.1
3	X	115	VAL	4.1
3	G	134	CYS	4.1
1	S	453	ILE	4.1
3	U	191	VAL	4.1
3	R	92	ILE	4.1
4	H	67	VAL	4.1
4	J	181	VAL	4.1
1	P	58	ALA	4.1
1	P	283	ASN	4.1
1	I	338	TRP	4.1
1	S	452	LEU	4.1
4	W	141	LEU	4.1
4	Q	91	PHE	4.1
1	P	349	LEU	4.1
4	J	93	ALA	4.0
1	A	338	TRP	4.0
3	U	196	VAL	4.0
3	O	1	ASP	4.0
1	M	453	ILE	4.0
1	A	361	PHE	4.0
3	K	148	TRP	4.0
4	J	73	MET	4.0
3	L	29	ILE	4.0
1	B	45	TRP	4.0
3	L	118	PHE	4.0
1	I	284	ILE	4.0
4	J	82	LEU	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	R	17	ASP	4.0
1	B	468	PHE	4.0
1	S	58	ALA	4.0
1	B	339	ASN	4.0
4	J	189	LEU	4.0
1	B	333	VAL	3.9
1	S	82	GLN	3.9
4	C	182	VAL	3.9
1	A	349	LEU	3.9
3	X	11	VAL	3.9
4	N	4	LEU	3.9
4	W	122	PHE	3.9
3	O	84	ALA	3.9
4	C	137	ALA	3.9
3	L	33	LEU	3.9
4	H	137	ALA	3.9
3	G	62	PHE	3.9
4	N	146	PHE	3.9
3	R	153	ALA	3.9
1	A	468	PHE	3.9
1	E	301	ASN	3.9
3	L	149	LYS	3.9
4	T	100(C)	PHE	3.9
1	I	60	ALA	3.8
2	v	27	VAL	3.8
4	J	190	GLY	3.8
3	K	83	PHE	3.8
4	N	207	VAL	3.8
1	B	420	ILE	3.8
4	Q	11	LEU	3.8
4	T	11	LEU	3.8
4	T	189	LEU	3.8
3	U	180	THR	3.8
4	Q	126	PRO	3.8
1	V	349	LEU	3.8
4	N	12	LEU	3.8
4	J	102	PRO	3.8
4	N	127	SER	3.8
3	L	209	PHE	3.8
3	U	161	GLU	3.8
4	J	10	GLY	3.7
3	O	191	VAL	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	C	20	LEU	3.7
4	J	167	PRO	3.7
4	N	142	VAL	3.7
3	R	194	CYS	3.7
3	K	143	GLU	3.7
3	D	133	VAL	3.7
4	C	38	ARG	3.7
4	F	110	THR	3.7
3	K	132	VAL	3.7
3	D	33	LEU	3.7
3	G	179	LEU	3.7
3	K	190	LYS	3.7
3	D	204	PRO	3.7
1	V	374	HIS	3.7
4	N	67	VAL	3.7
4	W	124	LEU	3.7
3	O	35	TRP	3.7
3	D	114	SER	3.7
4	W	125	ALA	3.7
3	D	116	PHE	3.7
4	F	34	TRP	3.7
1	I	335	GLY	3.6
4	F	130	SER	3.6
1	M	346	VAL	3.6
1	M	217	TYR	3.6
1	B	284	ILE	3.6
4	F	91	PHE	3.6
3	D	203	SER	3.6
4	J	45	LEU	3.6
1	V	408	SER	3.6
1	E	282	LYS	3.6
1	M	261	LEU	3.6
3	X	104	LEU	3.6
1	P	100	MET	3.6
3	K	110	VAL	3.6
4	Q	20	LEU	3.6
4	T	59	TYR	3.6
1	A	288	LEU	3.6
3	R	136	LEU	3.6
1	P	213	ILE	3.6
3	R	147	GLN	3.6
4	W	113	SER	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	G	210	ASN	3.6
1	I	454	LEU	3.6
4	W	80	LEU	3.6
3	D	124	GLN	3.6
1	P	285	ILE	3.5
3	K	162	SER	3.5
4	W	129	LYS	3.5
3	X	77	SER	3.5
3	U	118	PHE	3.5
3	X	102	THR	3.5
4	C	135	THR	3.5
4	N	152	VAL	3.5
3	X	33	LEU	3.5
1	V	285	ILE	3.5
4	W	114	ALA	3.5
3	K	22	THR	3.5
4	N	131	THR	3.5
3	D	137	ASN	3.5
1	S	381	GLU	3.5
1	S	287	GLN	3.5
1	S	468	PHE	3.5
1	M	272	ILE	3.5
4	F	205	THR	3.5
4	N	14	PRO	3.5
1	B	405	GLY	3.5
3	O	194	CYS	3.5
3	D	82	ASP	3.5
4	J	193	THR	3.4
3	G	141	PRO	3.4
3	R	161	GLU	3.4
4	C	19	SER	3.4
1	S	342	LEU	3.4
1	B	294	ILE	3.4
3	U	78	LEU	3.4
1	P	322	SER	3.4
1	M	451	GLY	3.4
3	K	86	TYR	3.4
3	O	21	ILE	3.4
4	H	198	VAL	3.4
4	W	210	LYS	3.4
3	R	117	ILE	3.4
4	J	98	TRP	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	342	LEU	3.4
3	X	178	THR	3.4
4	F	68	THR	3.4
3	K	193	ALA	3.4
4	F	213	PRO	3.4
4	Q	214	LYS	3.4
3	K	80	PRO	3.3
3	L	201	LEU	3.3
4	F	18	LEU	3.3
3	K	163	VAL	3.3
3	O	122	ASP	3.3
4	Q	71	LEU	3.3
4	H	126	PRO	3.3
1	E	338	TRP	3.3
3	R	46	LEU	3.3
4	J	115	SER	3.3
3	O	133	VAL	3.3
1	E	56	SER	3.3
3	X	47	VAL	3.3
4	F	87	THR	3.3
3	G	105	GLU	3.3
4	J	158	ALA	3.3
4	W	140	CYS	3.3
3	K	153	ALA	3.3
4	N	87	THR	3.3
4	J	106	GLY	3.3
1	I	406	THR	3.3
4	N	91	PHE	3.3
3	G	31	SER	3.3
4	N	140	CYS	3.3
3	D	117	ILE	3.3
3	O	129	THR	3.3
3	O	196	VAL	3.3
4	F	194	TYR	3.2
2	m	26	CYS	3.2
3	R	183	LYS	3.2
3	R	115	VAL	3.2
3	O	181	LEU	3.2
3	X	60	SER	3.2
4	W	154	TRP	3.2
3	X	19	VAL	3.2
1	E	342	LEU	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	R	1	ASP	3.2
4	C	9	ALA	3.2
3	O	79	GLN	3.2
3	L	130	ALA	3.2
3	X	130	ALA	3.2
4	H	190	GLY	3.2
4	C	170	LEU	3.2
3	G	144	ALA	3.2
1	V	414	ILE	3.2
1	E	350	ARG	3.2
1	V	410	GLU	3.2
3	R	130	ALA	3.1
3	O	85	THR	3.1
4	F	178	LEU	3.1
4	N	147	PRO	3.1
1	P	468	PHE	3.1
3	K	17	ASP	3.1
4	T	137	ALA	3.1
4	W	48	ILE	3.1
1	P	470	PRO	3.1
1	S	361	PHE	3.1
4	C	124	LEU	3.1
1	E	346	VAL	3.1
1	P	286	VAL	3.1
3	K	126	LYS	3.1
1	E	361	PHE	3.1
1	S	242	VAL	3.1
4	C	207	VAL	3.1
4	T	150	VAL	3.1
4	T	154	TRP	3.1
4	J	187	SER	3.1
4	Q	132	SER	3.1
4	T	50	GLU	3.1
1	I	452	LEU	3.1
3	X	185	ASP	3.1
4	W	109	VAL	3.1
1	S	374	HIS	3.1
4	Q	34	TRP	3.1
1	E	492	GLU	3.1
4	H	71	LEU	3.1
4	C	193	THR	3.1
4	Q	54	ASN	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	J	92	CYS	3.1
4	Q	98	TRP	3.1
4	W	34	TRP	3.1
1	S	49	ASN	3.1
2	v	17	GLY	3.1
4	F	212	GLU	3.1
3	K	10	PHE	3.1
4	H	132	SER	3.0
4	W	91	PHE	3.0
1	B	457	ASP	3.0
1	E	83	GLU	3.0
4	N	206	LYS	3.0
3	D	87	TYR	3.0
4	H	140	CYS	3.0
1	M	220	PRO	3.0
4	W	212	GLU	3.0
3	U	86	TYR	3.0
1	M	483	LEU	3.0
3	X	187	GLU	3.0
4	W	100(C)	PHE	3.0
1	P	49	ASN	3.0
4	N	161	SER	3.0
4	F	92	CYS	3.0
1	I	408	SER	3.0
1	E	383	PHE	3.0
4	F	38	ARG	3.0
3	O	13	ALA	3.0
4	N	159	LEU	3.0
3	G	2	ILE	3.0
1	B	349	LEU	3.0
1	M	454	LEU	3.0
4	F	115	SER	3.0
4	N	180	SER	3.0
1	V	60	ALA	3.0
4	Q	45	LEU	3.0
3	X	167	ASP	3.0
1	V	342	LEU	3.0
4	H	100(C)	PHE	3.0
1	V	286	VAL	3.0
4	J	150	VAL	3.0
3	K	187	GLU	3.0
1	E	50	THR	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	R	148	TRP	3.0
1	V	49	ASN	3.0
4	Q	175	LEU	3.0
4	T	95	ARG	2.9
4	J	111	VAL	2.9
3	U	127	SER	2.9
1	V	100	MET	2.9
4	T	185	PRO	2.9
1	I	324	GLY	2.9
3	O	193	ALA	2.9
4	J	48	ILE	2.9
1	M	100	MET	2.9
4	N	148	GLU	2.9
3	X	134	CYS	2.9
3	X	208	SER	2.9
4	J	186	SER	2.9
3	G	143	GLU	2.9
3	D	200	GLY	2.9
3	O	105	GLU	2.9
4	W	173	SER	2.9
1	S	349	LEU	2.9
4	F	95	ARG	2.9
4	W	20	LEU	2.9
4	H	59	TYR	2.9
4	N	17	THR	2.9
3	G	48	ILE	2.9
4	N	149	PRO	2.9
3	R	179	LEU	2.9
4	J	124	LEU	2.9
1	M	487	LYS	2.9
3	L	168	SER	2.9
4	H	4	LEU	2.9
4	C	179	SER	2.9
4	Q	82	LEU	2.9
3	O	102	THR	2.9
3	O	206	THR	2.9
3	D	78	LEU	2.9
3	O	117	ILE	2.9
4	J	78	PHE	2.9
4	J	142	VAL	2.9
1	B	285	ILE	2.9
3	X	61	ARG	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	X	46	LEU	2.9
4	T	213	PRO	2.9
4	C	98	TRP	2.9
4	W	152	VAL	2.9
1	M	342	LEU	2.9
4	Q	48	ILE	2.9
3	R	113	PRO	2.8
3	R	55	GLN	2.8
4	T	184	VAL	2.8
1	S	288	LEU	2.8
1	S	390	LEU	2.8
3	X	87	TYR	2.8
3	X	118	PHE	2.8
4	J	138	LEU	2.8
1	E	488	VAL	2.8
3	K	202	SER	2.8
4	F	132	SER	2.8
4	J	95	ARG	2.8
1	E	381	GLU	2.8
1	P	217	TYR	2.8
3	L	158	ASN	2.8
4	T	57	PRO	2.8
4	J	21	THR	2.8
1	I	349	LEU	2.8
3	X	149	LYS	2.8
3	O	148	TRP	2.8
3	X	183	LYS	2.8
1	B	240	LYS	2.8
1	A	381	GLU	2.8
1	S	272	ILE	2.8
4	T	69	ILE	2.8
3	G	104	LEU	2.8
4	H	69	ILE	2.8
3	R	27	GLN	2.8
4	C	34	TRP	2.8
4	Q	108	LEU	2.8
3	O	205	VAL	2.8
3	U	110	VAL	2.8
4	H	180	SER	2.8
3	U	21	ILE	2.8
4	F	184	VAL	2.8
1	E	288	LEU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	C	80	LEU	2.8
3	D	186	TYR	2.7
3	D	182	SER	2.7
4	F	214	LYS	2.7
1	V	381	GLU	2.7
4	F	33	TYR	2.7
4	N	194	TYR	2.7
4	W	11	LEU	2.7
3	X	75	ILE	2.7
4	W	17	THR	2.7
3	K	195	GLU	2.7
3	X	122	ASP	2.7
1	E	217	TYR	2.7
3	G	129	THR	2.7
4	Q	165	THR	2.7
1	E	49	ASN	2.7
3	L	196	VAL	2.7
3	D	47	VAL	2.7
4	C	10	GLY	2.7
4	Q	106	GLY	2.7
3	L	132	VAL	2.7
3	X	142	ARG	2.7
4	N	141	LEU	2.7
1	A	345	VAL	2.7
3	O	146	VAL	2.7
4	N	150	VAL	2.7
3	X	165	GLU	2.7
4	J	141	LEU	2.7
3	U	117	ILE	2.7
3	K	151	ASP	2.7
3	R	154	LEU	2.7
3	X	94	LEU	2.7
1	B	454	LEU	2.7
4	H	29	LEU	2.7
4	J	91	PHE	2.7
4	W	4	LEU	2.7
4	W	123	PRO	2.7
4	H	179	SER	2.7
3	L	38	GLN	2.7
1	I	361	PHE	2.7
2	i	18	ARG	2.7
3	X	182	SER	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	409	ILE	2.7
3	X	198	HIS	2.7
3	X	125	LEU	2.6
1	M	253	PRO	2.6
3	O	36	TYR	2.6
1	V	217	TYR	2.6
3	D	145	LYS	2.6
3	O	40	PRO	2.6
1	I	345	VAL	2.6
1	B	470	PRO	2.6
3	D	19	VAL	2.6
1	B	492	GLU	2.6
3	X	124	GLN	2.6
1	S	284	ILE	2.6
4	H	45	LEU	2.6
1	B	392	ASN	2.6
3	D	14	SER	2.6
3	D	163	VAL	2.6
4	H	111	VAL	2.6
4	Q	184	VAL	2.6
2	v	18	ARG	2.6
3	G	166	GLN	2.6
3	K	29	ILE	2.6
4	W	120	SER	2.6
1	E	69	TRP	2.6
4	W	159	LEU	2.6
4	T	210	LYS	2.6
1	M	288	LEU	2.6
3	G	180	THR	2.6
4	J	152	VAL	2.6
3	X	144	ALA	2.6
3	G	142	ARG	2.6
1	E	93	PHE	2.6
1	E	423	ILE	2.5
1	M	52	LEU	2.5
3	L	117	ILE	2.5
3	K	201	LEU	2.5
3	R	186	TYR	2.5
3	K	118	PHE	2.5
3	K	207	LYS	2.5
2	b	27	VAL	2.5
4	W	196	CYS	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	U	35	TRP	2.5
1	B	443	ILE	2.5
3	D	177	SER	2.5
1	B	472	GLY	2.5
4	H	139	GLY	2.5
4	N	125	ALA	2.5
1	E	107	ASP	2.5
4	H	3	GLN	2.5
3	R	175	LEU	2.5
4	T	183	THR	2.5
3	U	33	LEU	2.5
3	X	120	PRO	2.5
4	W	162	GLY	2.5
3	D	151	ASP	2.5
4	C	110	THR	2.5
3	O	190	LYS	2.5
4	T	119	PRO	2.5
3	K	192	TYR	2.5
1	I	341	THR	2.5
4	F	103	TRP	2.5
1	M	374	HIS	2.5
4	J	90	TYR	2.5
1	E	477	ASP	2.5
1	E	272	ILE	2.5
4	C	132	SER	2.5
4	F	121	VAL	2.5
1	A	324	GLY	2.5
3	D	194	CYS	2.5
3	G	152	ASN	2.5
4	Q	207	VAL	2.5
4	T	27	GLU	2.5
4	C	136	ALA	2.5
3	G	197	THR	2.5
3	X	20	THR	2.5
4	N	70	SER	2.5
1	V	471	GLY	2.5
3	G	54	LEU	2.5
4	F	80	LEU	2.5
1	S	93	PHE	2.5
4	J	126	PRO	2.5
4	F	170	LEU	2.5
1	B	60	ALA	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	R	126	LYS	2.5
1	B	87	GLU	2.4
3	X	81	GLU	2.4
3	G	115	VAL	2.4
1	B	486	TYR	2.4
4	W	68	THR	2.4
3	K	48	ILE	2.4
3	U	123	GLU	2.4
4	J	140	CYS	2.4
4	Q	181	VAL	2.4
4	H	130	SER	2.4
4	N	132	SER	2.4
4	W	183	THR	2.4
1	E	376	PHE	2.4
4	C	209	LYS	2.4
4	C	69	ILE	2.4
3	X	116	PHE	2.4
4	F	98	TRP	2.4
1	A	346	VAL	2.4
1	B	46	LYS	2.4
3	O	186	TYR	2.4
4	H	95	ARG	2.4
1	P	420	ILE	2.4
3	X	166	GLN	2.4
4	N	157	GLY	2.4
1	A	259	LEU	2.4
4	T	194	TYR	2.4
3	K	55	GLN	2.4
4	N	68	THR	2.4
3	R	2	ILE	2.4
4	C	195	ILE	2.4
1	E	345	VAL	2.4
3	K	1	ASP	2.4
4	J	67	VAL	2.4
1	E	468	PHE	2.4
3	D	107	LYS	2.4
3	K	179	LEU	2.4
4	W	214	LYS	2.4
3	D	143	GLU	2.4
4	W	81	ASN	2.4
3	U	141	PRO	2.4
3	K	123	GLU	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	90	TYR	2.4
4	J	173	SER	2.4
1	A	351	LYS	2.4
1	B	282	LYS	2.4
3	X	153	ALA	2.4
1	P	333	VAL	2.4
3	X	40	PRO	2.4
4	T	37	VAL	2.4
4	C	12	LEU	2.4
1	B	477	ASP	2.4
4	N	37	VAL	2.4
1	P	253	PRO	2.4
3	U	62	PHE	2.4
2	v	16	LEU	2.4
4	J	100(C)	PHE	2.4
1	M	390	LEU	2.4
4	N	124	LEU	2.4
4	N	178	LEU	2.4
4	Q	92	CYS	2.4
1	M	406	THR	2.4
2	s	18	ARG	2.3
4	J	155	ASN	2.3
1	M	345	VAL	2.3
4	W	142	VAL	2.3
4	W	198	VAL	2.3
1	M	486	TYR	2.3
4	H	78	PHE	2.3
4	Q	115	SER	2.3
1	P	405	GLY	2.3
3	O	179	LEU	2.3
4	Q	121	VAL	2.3
1	E	287	GLN	2.3
1	E	451	GLY	2.3
2	m	27	VAL	2.3
4	C	141	LEU	2.3
1	I	381	GLU	2.3
1	P	259	LEU	2.3
3	X	73	LEU	2.3
4	Q	170	LEU	2.3
4	W	50	GLU	2.3
1	A	271	MET	2.3
4	H	181	VAL	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	I	288	LEU	2.3
1	P	342	LEU	2.3
3	G	126	LYS	2.3
4	C	214	LYS	2.3
1	A	454	LEU	2.3
2	a	18	ARG	2.3
4	F	126	PRO	2.3
3	U	198	HIS	2.3
1	E	91	GLU	2.3
3	L	136	LEU	2.3
3	O	94	LEU	2.3
4	C	107	THR	2.3
4	F	189	LEU	2.3
1	I	300	ASN	2.3
4	Q	97	ASN	2.3
4	F	71	LEU	2.3
4	N	29	LEU	2.3
3	U	143	GLU	2.3
1	I	471	GLY	2.3
1	I	270	VAL	2.3
4	N	27	GLU	2.3
1	P	361	PHE	2.3
1	I	486	TYR	2.3
1	I	453	ILE	2.3
3	K	91	LEU	2.3
4	H	129	LYS	2.3
1	S	81	PRO	2.3
3	R	124	GLN	2.3
4	C	198	VAL	2.3
4	Q	46	GLU	2.3
4	C	134	GLY	2.3
4	Q	55	GLY	2.3
1	E	105	HIS	2.3
4	F	164	HIS	2.3
3	X	209	PHE	2.3
3	O	143	GLU	2.2
3	K	35	TRP	2.2
3	R	78	LEU	2.2
1	B	78	ASP	2.2
3	X	48	ILE	2.2
3	X	154	LEU	2.2
3	X	201	LEU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	419	ARG	2.2
3	O	26	SER	2.2
4	J	184	VAL	2.2
1	B	80	SER	2.2
4	Q	70	SER	2.2
4	W	35	SER	2.2
4	C	59	TYR	2.2
1	I	492	GLU	2.2
3	K	137	ASN	2.2
1	B	406	THR	2.2
3	X	164	THR	2.2
4	J	80	LEU	2.2
4	T	124	LEU	2.2
1	B	79	PRO	2.2
1	A	482	GLU	2.2
1	A	49	ASN	2.2
1	S	324	GLY	2.2
1	V	273	ARG	2.2
1	M	274	SER	2.2
3	D	183	LYS	2.2
3	O	20	THR	2.2
1	S	409	ILE	2.2
3	X	179	LEU	2.2
3	G	147	GLN	2.2
4	Q	1	GLN	2.2
3	X	86	TYR	2.2
4	T	200	HIS	2.2
1	M	381	GLU	2.2
4	Q	28	SER	2.2
4	J	209	LYS	2.2
1	M	416	LEU	2.2
2	e	22	THR	2.2
3	L	14	SER	2.2
3	D	127	SER	2.2
4	F	82	LEU	2.2
1	I	258	GLN	2.2
3	K	24	ARG	2.2
3	U	25	ALA	2.2
4	J	5	GLN	2.2
1	A	52	LEU	2.2
1	E	261	LEU	2.2
4	T	152	VAL	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	P	357	ASN	2.2
3	R	158	ASN	2.2
1	E	239	CYS	2.2
3	X	13	ALA	2.2
3	K	78	LEU	2.2
3	G	26	SER	2.2
4	F	131	THR	2.2
4	Q	183	THR	2.2
4	N	85	ALA	2.1
1	E	260	LEU	2.1
3	D	146	VAL	2.1
4	J	127	SER	2.1
4	N	186	SER	2.1
4	T	35	SER	2.1
3	X	123	GLU	2.1
3	G	205	VAL	2.1
3	O	19	VAL	2.1
4	Q	209	LYS	2.1
3	K	2	ILE	2.1
4	H	131	THR	2.1
1	I	344	GLN	2.1
1	M	273	ARG	2.1
3	D	142	ARG	2.1
4	T	143	LYS	2.1
4	N	151	THR	2.1
3	U	144	ALA	2.1
1	V	250	GLY	2.1
1	P	86	MET	2.1
3	D	34	ALA	2.1
4	F	152	VAL	2.1
1	P	381	GLU	2.1
3	L	147	GLN	2.1
4	C	73	MET	2.1
3	R	118	PHE	2.1
4	T	98	TRP	2.1
1	M	90	THR	2.1
1	P	407	ALA	2.1
3	G	199	GLN	2.1
4	H	107	THR	2.1
4	H	200	HIS	2.1
4	C	189	LEU	2.1
3	R	131	SER	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	F	113	SER	2.1
1	V	99	ASN	2.1
1	B	361	PHE	2.1
1	E	199	SER	2.1
4	N	166	PHE	2.1
1	A	121	GLN	2.1
3	R	177	SER	2.1
4	Q	180	SER	2.1
4	W	143	LYS	2.1
4	Q	68	THR	2.1
4	H	97	ASN	2.1
4	F	198	VAL	2.1
4	W	54	ASN	2.1
1	E	210	PHE	2.1
3	O	168	SER	2.1
1	P	299	PRO	2.1
4	T	121	VAL	2.1
1	S	301	ASN	2.1
3	U	112	ALA	2.1
4	H	34	TRP	2.1
3	X	146	VAL	2.1
4	J	151	THR	2.1
1	B	49	ASN	2.1
3	O	165	GLU	2.1
4	H	91	PHE	2.1
4	N	115	SER	2.1
4	J	196	CYS	2.1
3	U	201	LEU	2.0
1	M	383	PHE	2.0
1	M	481	SER	2.0
4	T	180	SER	2.0
4	W	180	SER	2.0
3	K	32	TYR	2.0
3	U	24	ARG	2.0
3	X	180	THR	2.0
1	A	226	LEU	2.0
3	L	163	VAL	2.0
4	T	55	GLY	2.0
4	J	202	PRO	2.0
4	N	48	ILE	2.0
1	I	217	TYR	2.0
3	O	211	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
3	U	126	LYS	2.0
1	B	82	GLN	2.0
4	C	8	GLY	2.0
3	X	152	ASN	2.0
4	T	48	ILE	2.0
3	K	208	SER	2.0
3	R	107	LYS	2.0
3	G	78	LEU	2.0
3	U	186	TYR	2.0
4	Q	18	LEU	2.0
4	Q	109	VAL	2.0
1	A	198	GLY	2.0
4	Q	31	GLY	2.0
4	H	9	ALA	2.0
1	A	93	PHE	2.0
1	M	49	ASN	2.0
4	W	64	LYS	2.0
4	W	70	SER	2.0
1	B	471	GLY	2.0
1	S	228	CYS	2.0
4	C	144	ASP	2.0
1	E	390	LEU	2.0
3	K	94	LEU	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	OAS	Q	30	6/10	0.68	0.32	246,262,273,274	0
4	OAS	W	30	9/10	0.69	0.38	201,211,216,219	0
2	U2X	e	23	19/20	0.77	0.40	175,179,184,185	0
2	U2X	p	23	19/20	0.77	0.39	106,113,127,130	0
2	U2X	b	23	19/20	0.79	0.39	131,154,176,177	0
4	OAS	J	30	6/10	0.81	0.12	164,236,245,246	0
4	OAS	N	30	6/10	0.82	0.18	179,233,246,251	0
4	OAS	F	30	6/10	0.82	0.13	248,273,281,281	0
2	U2X	i	23	19/20	0.84	0.42	133,139,150,152	0
2	U2X	s	23	19/20	0.84	0.36	146,152,160,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	U2X	a	23	19/20	0.84	0.44	130,136,145,145	0
4	OAS	T	30	9/10	0.85	0.23	156,170,195,200	0
4	OAS	H	30	9/10	0.87	0.14	172,176,180,182	0
2	U2X	m	23	19/20	0.91	0.34	155,164,181,184	0
2	U2X	v	23	19/20	0.92	0.34	146,156,181,182	0
4	OAS	C	30	9/10	0.92	0.29	155,165,179,180	0
2	DPR	p	21	7/8	0.93	0.25	123,126,133,136	0
2	DPR	i	21	7/8	0.94	0.27	136,137,141,144	0
2	DPR	b	21	7/8	0.94	0.18	165,166,170,173	0
2	DPR	s	21	7/8	0.94	0.19	151,152,155,158	0
2	DPR	a	21	7/8	0.95	0.16	146,147,150,151	0
2	DPR	v	21	7/8	0.95	0.40	170,171,176,180	0
2	DPR	m	21	7/8	0.97	0.27	173,175,182,187	0
2	DPR	e	21	7/8	0.98	0.34	176,177,180,182	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	I	502	14/15	0.57	0.43	183,189,198,199	0
5	NAG	E	502	14/15	0.74	0.28	190,201,211,212	0
5	NAG	P	502	14/15	0.75	0.26	208,216,230,231	0
5	NAG	B	501	14/15	0.80	0.27	152,161,168,170	0
5	NAG	I	504	14/15	0.81	0.27	176,180,185,186	0
5	NAG	A	504	14/15	0.84	0.14	184,188,192,195	0
5	NAG	E	501	14/15	0.84	0.38	204,207,209,209	0
5	NAG	S	501	14/15	0.84	0.36	154,162,168,171	0
5	NAG	I	503	14/15	0.86	0.21	194,202,208,209	0
5	NAG	M	501	14/15	0.86	0.42	178,180,182,185	0
5	NAG	B	502	14/15	0.86	0.13	219,232,245,249	0
5	NAG	A	501	14/15	0.86	0.36	127,136,143,144	0
5	NAG	S	502	14/15	0.86	0.18	230,238,252,259	0
5	NAG	A	502	14/15	0.88	0.20	184,189,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	S	503	14/15	0.88	0.29	202,210,214,216	0
5	NAG	A	503	14/15	0.89	0.35	152,167,177,182	0
5	NAG	I	501	14/15	0.92	0.23	161,165,172,173	0
5	NAG	P	501	14/15	0.92	0.22	153,165,177,177	0
5	NAG	V	501	14/15	0.94	0.38	153,158,163,165	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.