



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:19 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

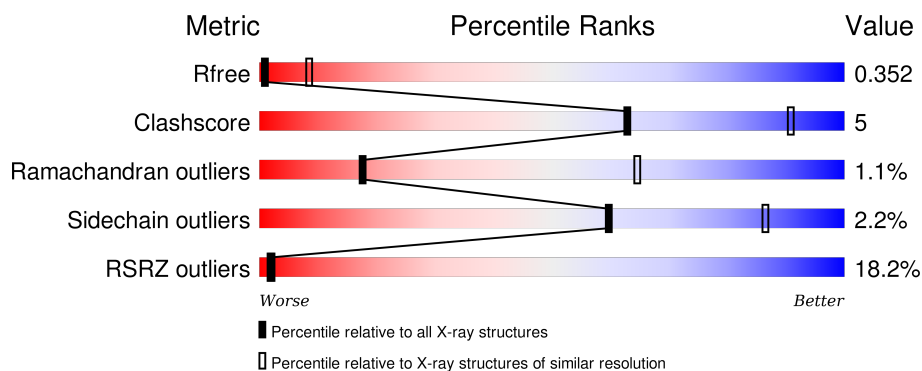
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.56 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}	91344	1240 (3.72-3.40)
Clashscore	102246	1057 (3.70-3.42)
Ramachandran outliers	100387	1017 (3.70-3.42)
Sidechain outliers	100360	1017 (3.70-3.42)
RSRZ outliers	91569	1247 (3.72-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	352	<div> <div>9%</div> <div>87%</div> <div>7%</div> <div>5%</div> </div>
1	B	352	<div> <div>12%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
1	E	352	<div> <div>14%</div> <div>87%</div> <div>6%</div> <div>• 7%</div> </div>
1	I	352	<div> <div>8%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
1	M	352	<div> <div>12%</div> <div>88%</div> <div>8%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

2 Entry composition

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

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

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

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

- Molecule 2 is a protein called M48U1 peptide.

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

Continued on next page...

Continued from previous page...

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

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

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

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

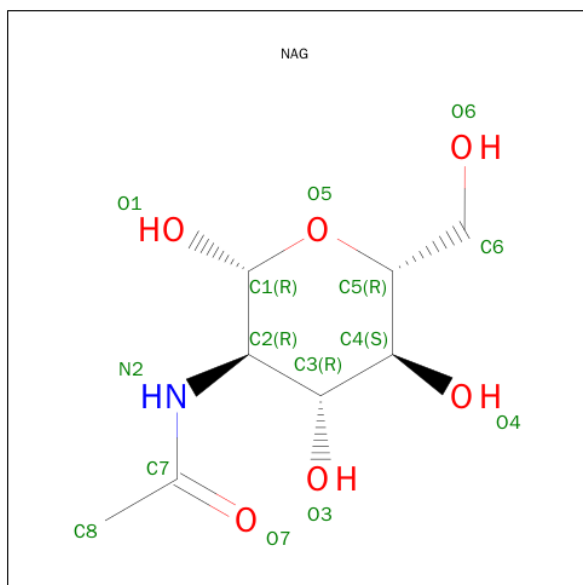
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	220	Total 3322	C 1066	H 1648	N 283	O 320	S 5	0	0	0
4	C	220	Total 3245	C 1066	H 1571	N 283	O 320	S 5	0	0	0
4	F	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	J	220	Total 3186	C 1064	H 1515	N 283	O 319	S 5	0	0	0
4	N	220	Total 3322	C 1064	H 1651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

Continued on next page...

Continued from previous page...

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

Continued on next page...

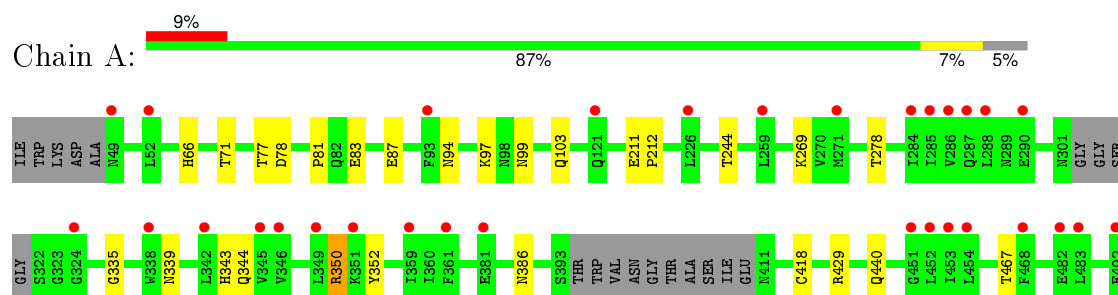
Continued from previous page...

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

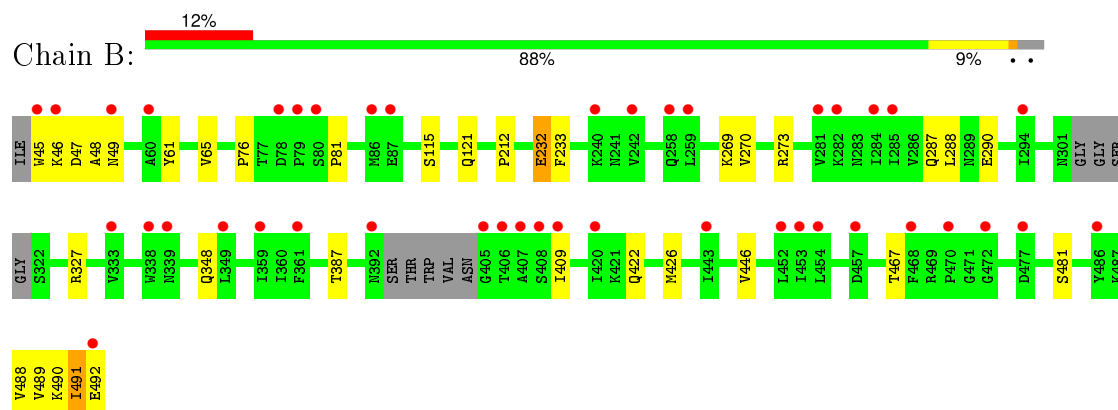
3 Residue-property plots [i](#)

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

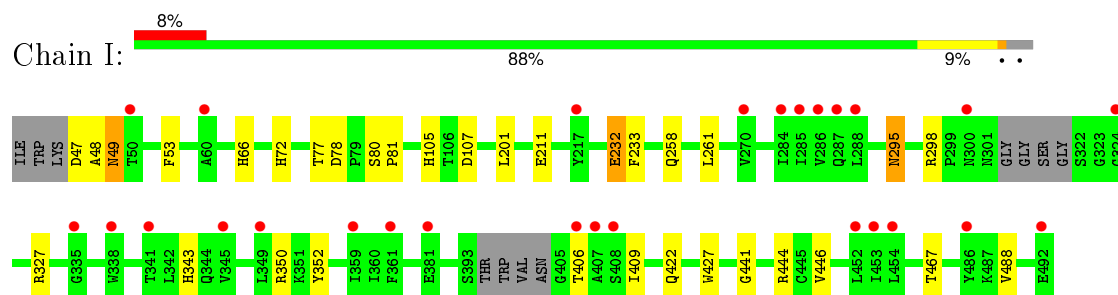
• Molecule 1: HIV-1 gp120



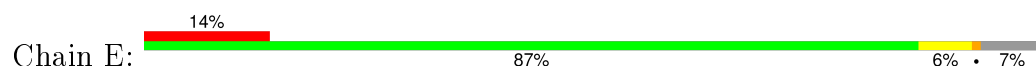
• Molecule 1: HIV-1 gp120

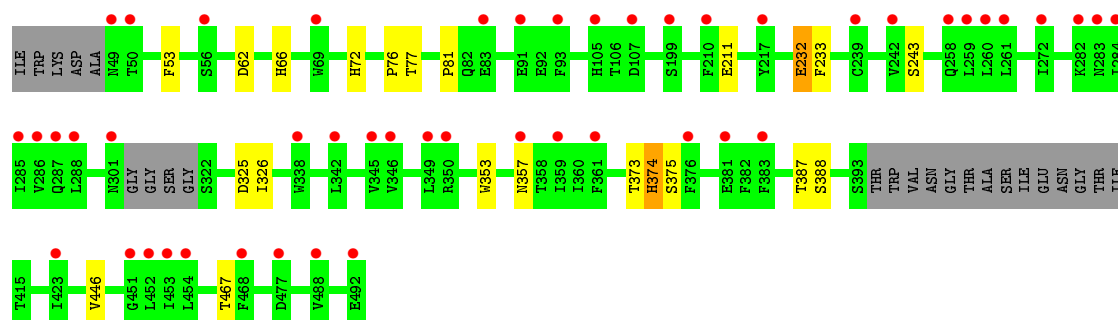


• Molecule 1: HIV-1 gp120

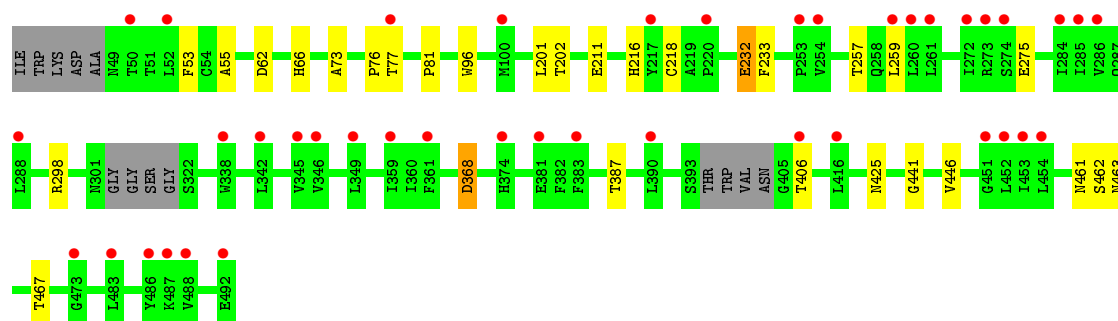
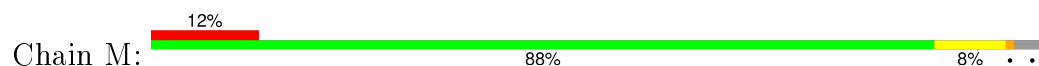


• Molecule 1: HIV-1 gp120

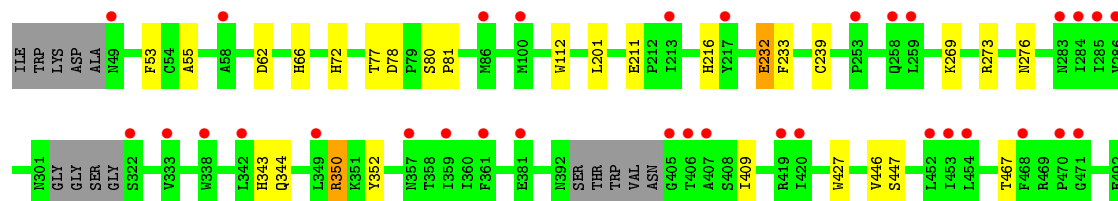
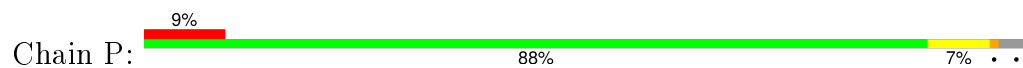




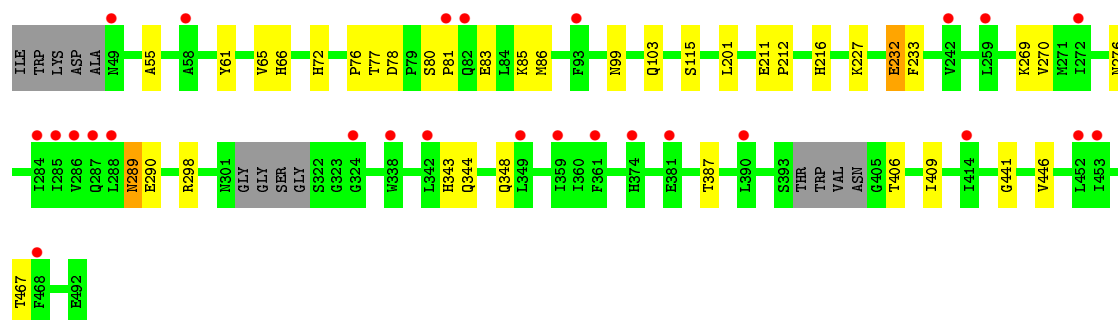
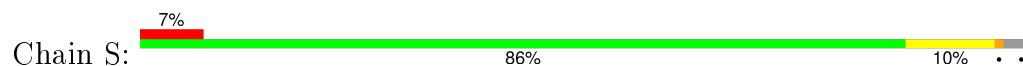
- Molecule 1: HIV-1 gp120



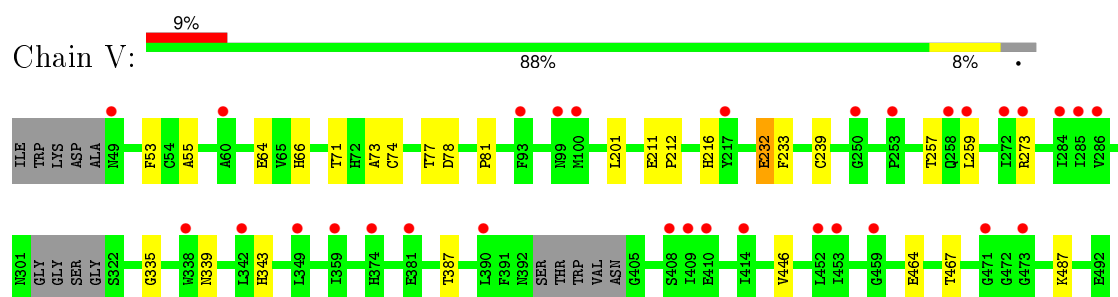
- Molecule 1: HIV-1 gp120



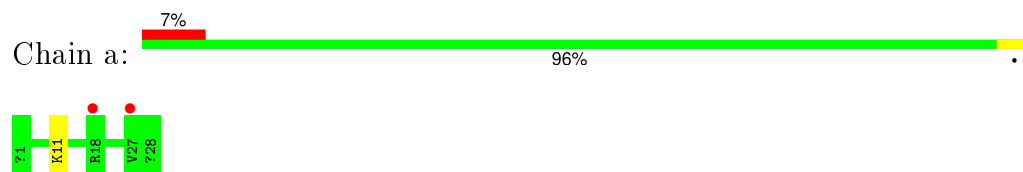
- Molecule 1: HIV-1 gp120



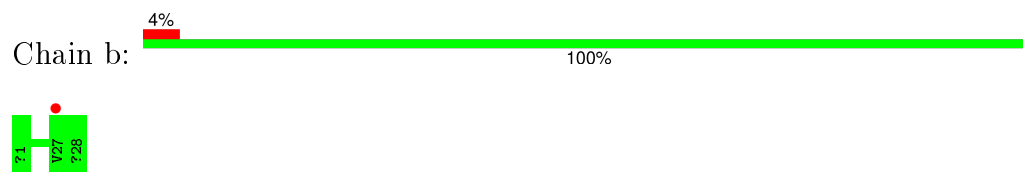
- Molecule 1: HIV-1 gp120



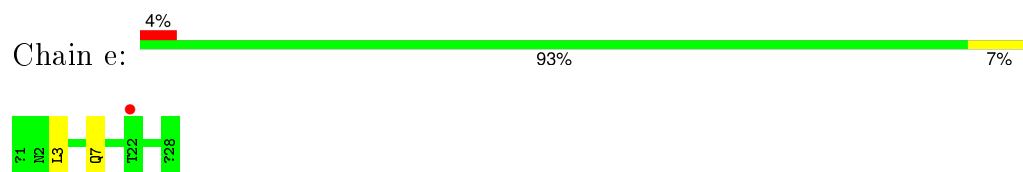
- Molecule 2: M48U1 peptide



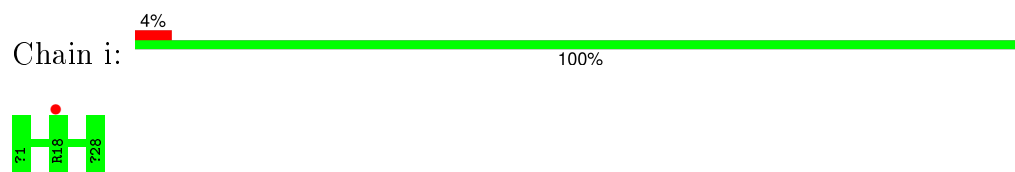
- Molecule 2: M48U1 peptide



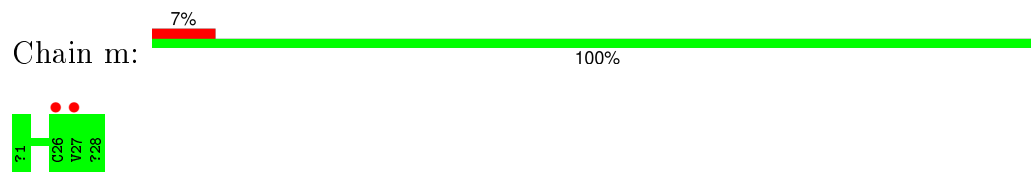
- Molecule 2: M48U1 peptide



- Molecule 2: M48U1 peptide

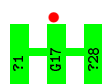


- Molecule 2: M48U1 peptide



- Molecule 2: M48U1 peptide

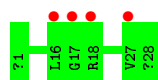




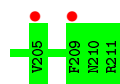
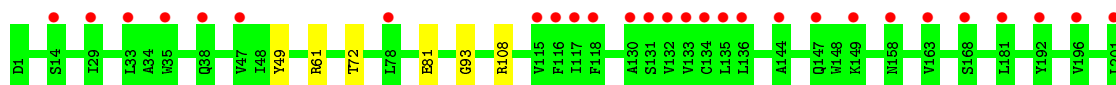
- Molecule 2: M48U1 peptide



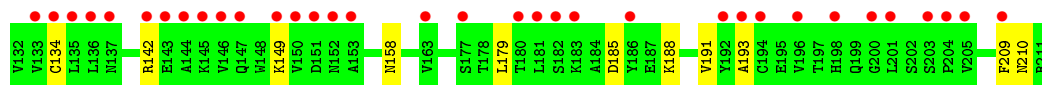
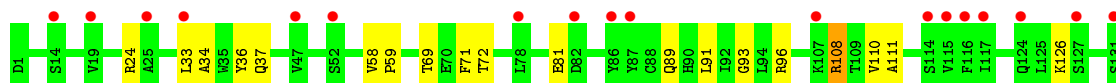
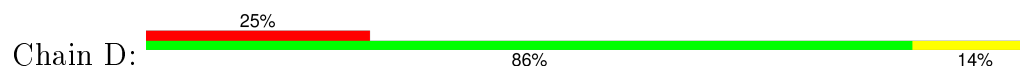
- Molecule 2: M48U1 peptide



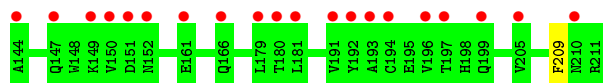
- Molecule 3: Antibody 2.2c LIGHT CHAIN



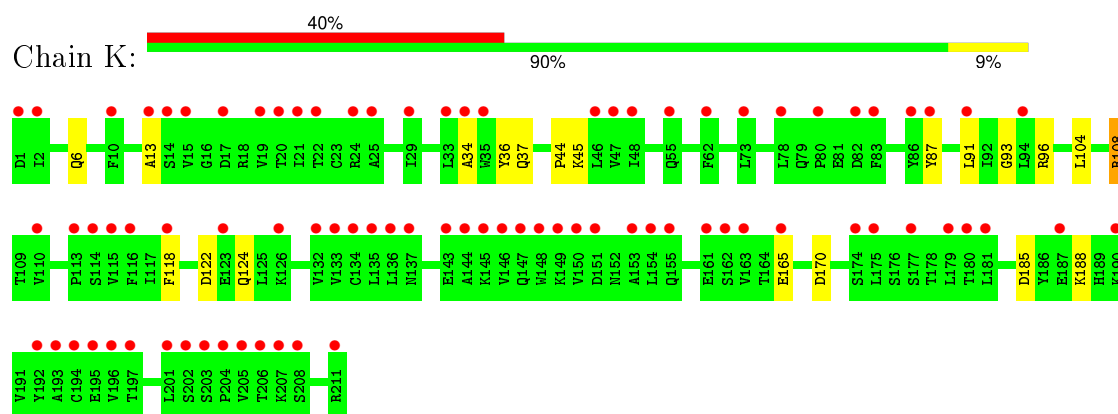
- Molecule 3: Antibody 2.2c LIGHT CHAIN



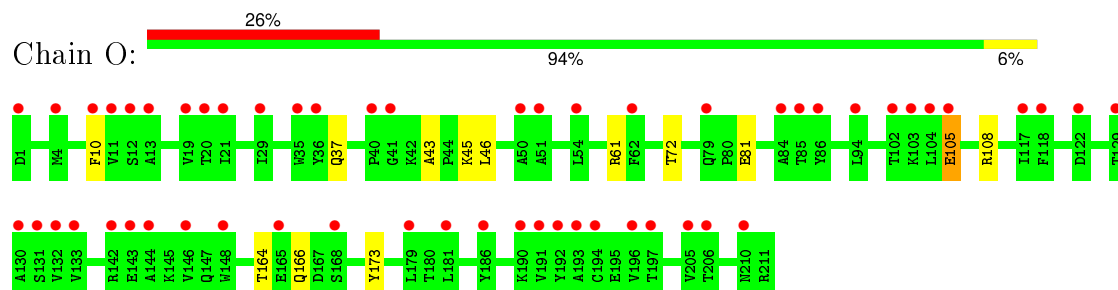
- Molecule 3: Antibody 2.2c LIGHT CHAIN



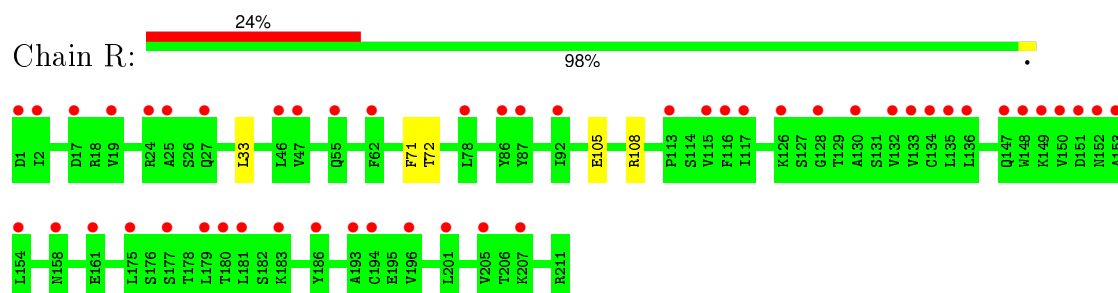
- Molecule 3: Antibody 2.2c LIGHT CHAIN



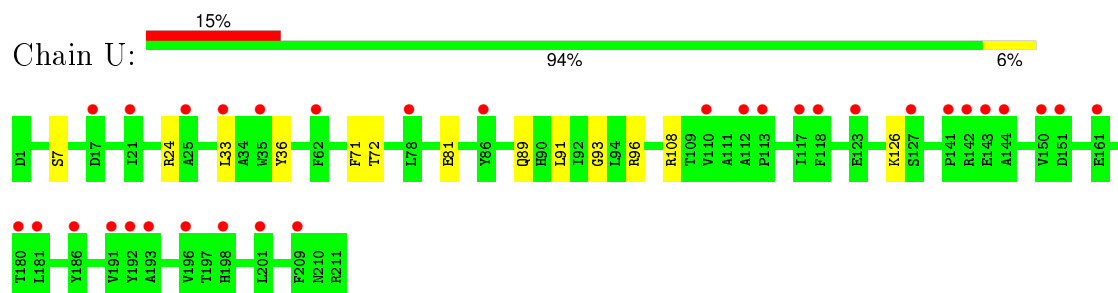
• Molecule 3: Antibody 2.2c LIGHT CHAIN



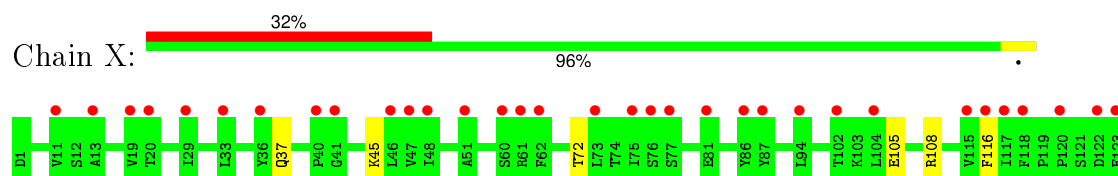
• Molecule 3: Antibody 2.2c LIGHT CHAIN

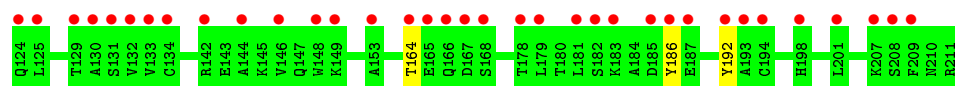


• Molecule 3: Antibody 2.2c LIGHT CHAIN

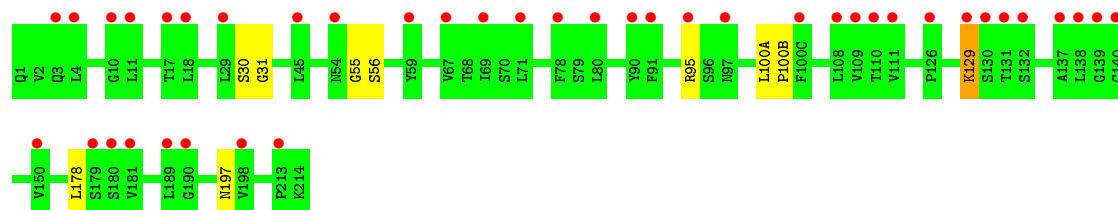


• Molecule 3: Antibody 2.2c LIGHT CHAIN

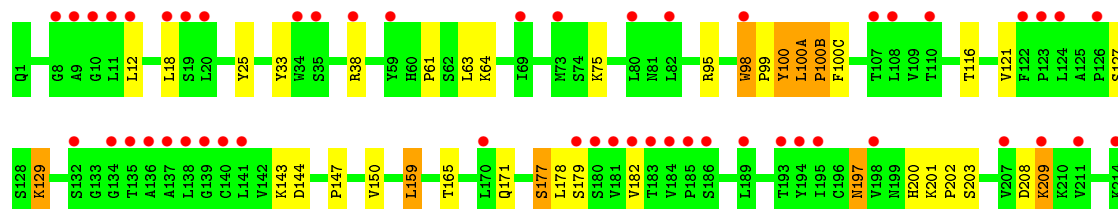
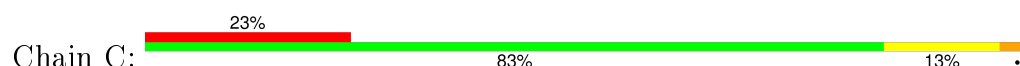




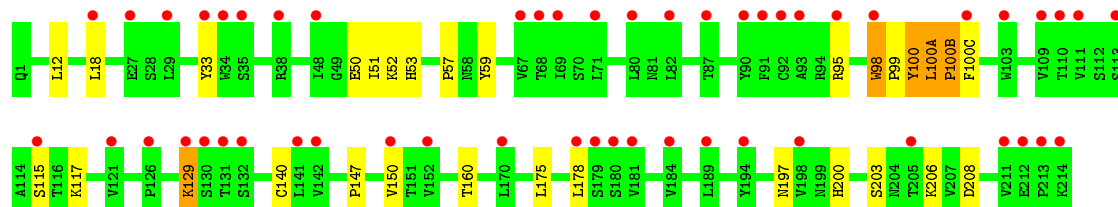
• Molecule 4: Antibody 2.2c heavy CHAIN



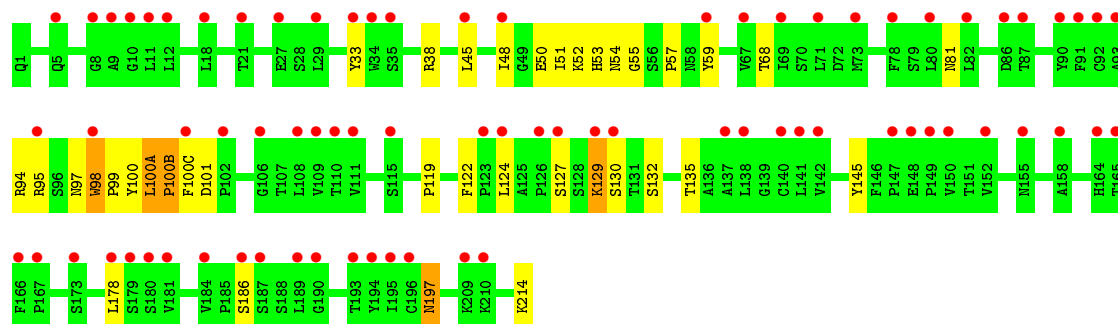
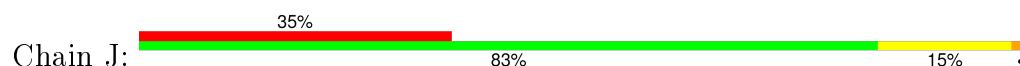
• Molecule 4: Antibody 2.2c heavy CHAIN



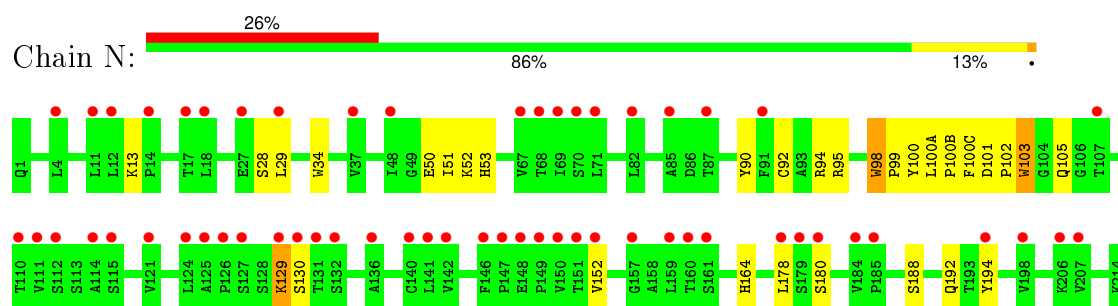
• Molecule 4: Antibody 2.2c heavy CHAIN



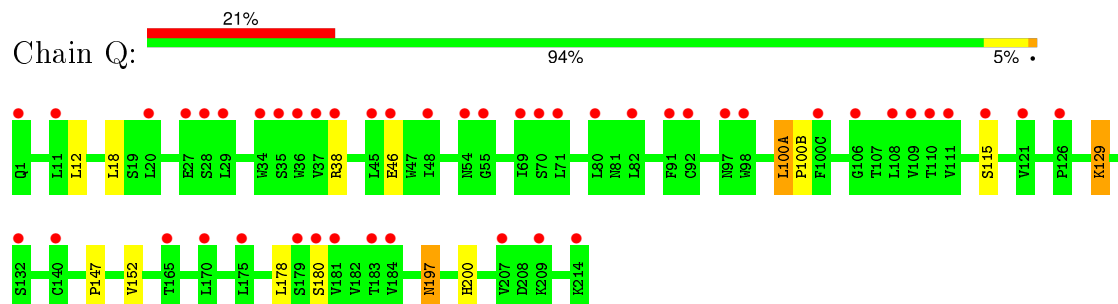
• Molecule 4: Antibody 2.2c heavy CHAIN



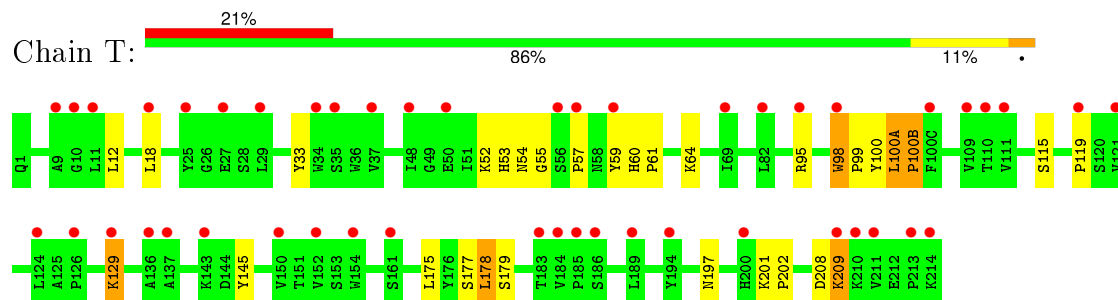
• Molecule 4: Antibody 2.2c heavy CHAIN



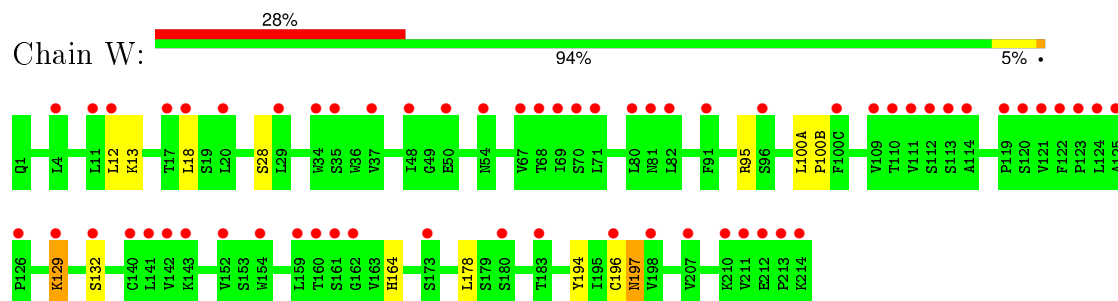
- Molecule 4: Antibody 2.2c heavy CHAIN



- 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, α , β , γ	112.97Å 144.18Å 158.35Å 110.58° 92.30° 99.19°	Depositor
Resolution (Å)	49.15 – 3.56 49.15 – 2.85	Depositor EDS
% Data completeness (in resolution range)	62.7 (49.15-3.56) 33.5 (49.15-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.296 , 0.328 0.322 , 0.352	Depositor DCC
R_{free} test set	3546 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	99.3	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 160.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 71729 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	94738	wwPDB-VP
Average B, all atoms (Å ²)	217.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

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

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1
4	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
4:J:95:ARG:NH2	4:J:100(A):LEU:HD13	2.00	0.76
3:D:91:LEU:CD2	4:C:100(B):PRO:HB3	2.15	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
4:F:98:TRP:H	4:F:99:PRO:CA	2.04	0.71
1:A:212:PRO:HG3	5:A:501:NAG:H2	1.70	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
4:T:100(A):LEU:HB3	4:T:100(B):PRO:CA	2.16	0.69
1:I:295:ASN:N	1:I:295:ASN:OD1	2.24	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

Continued on next page...

Continued from previous page...

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
3:K:91:LEU:HD22	4:J:100(A):LEU:HB2	1.75	0.67
1:B:491:ILE:HG22	1:B:492:GLU:HG3	1.75	0.67
1:B:446:VAL:O	5:B:501:NAG:H5	1.95	0.67
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
4:Q:147:PRO:O	4:Q:200:HIS:NE2	2.30	0.65
1:M:232:GLU:CB	1:M:233:PHE:HA	2.27	0.65
3:G:62:PHE:CE2	3:G:75:ILE:HD11	2.31	0.65
1:B:121:GLN:NE2	1:B:426:MET:SD	2.69	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:S:270:VAL:O	1:S:348:GLN:NE2	2.31	0.62
1:E:232:GLU:CB	1:E:233:PHE:HA	2.28	0.62
4:J:95:ARG:HH21	4:J:100(A):LEU:HD13	1.62	0.62
4:F:100(A):LEU:CB	4:F:100(B):PRO:HA	2.22	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
1:P:232:GLU:CB	1:P:233:PHE:HA	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:117:LYS:HB2	3:U:126:LYS:HZ2	1.64	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:T:98:TRP:N	4:T:99:PRO:HA	2.12	0.61
4:J:98:TRP:HB3	4:J:100:TYR:HB2	1.81	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:P:344:GLN:OE1	5:P:502:NAG:H62	2.01	0.59
1:I:232:GLU:CB	1:I:233:PHE:HA	2.31	0.59
4:J:52:LYS:HG3	4:J:54:ASN:H	1.68	0.59
1:S:212:PRO:HG3	5:S:501:NAG:H2	1.84	0.59
4:J:57:PRO:HB2	4:J:59:TYR:CZ	2.38	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
4:F:95:ARG:NH2	4:F:100(A):LEU:HD13	2.19	0.57
1:I:327:ARG:NH2	1:I:422:GLN:OE1	2.37	0.57
1:E:353:TRP:O	1:E:357:ASN:ND2	2.36	0.57
1:S:348:GLN:HE21	5:S:502:NAG:H81	1.70	0.57
1:B:232:GLU:CB	1:B:233:PHE:HA	2.34	0.57
1:V:212:PRO:CG	5:V:501:NAG:H2	2.34	0.57
4:T:33:TYR:CE1	4:T:52:LYS:HB2	2.38	0.57
1:P:269:LYS:HE2	5:P:502:NAG:H4	1.87	0.57
1:V:66:HIS:ND1	1:V:211:GLU:O	2.38	0.57
3:K:93:GLY:O	3:K:96:ARG:NH1	2.34	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

Continued on next page...

Continued from previous page...

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:T:55:GLY:O	4:T:57:PRO:HD3	2.07	0.55
4:J:197:ASN:OD1	4:J:197:ASN:N	2.38	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
4:T:100(A):LEU:CB	4:T:100(B):PRO:CA	2.85	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: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
1:A:66:HIS:ND1	1:A:211:GLU:O	2.41	0.53
4:F:57:PRO:HB2	4:F:59:TYR:CE2	2.43	0.53
4:C:33:TYR:HB2	4:C:95:ARG:HB2	1.91	0.53
5:B:502:NAG:O3	5:B:502:NAG:O7	2.23	0.53
4:F:52:LYS:HG3	4:F:53:HIS:N	2.24	0.53
1:A:99:ASN:OD1	1:A:103:GLN:NE2	2.42	0.53
4:F:98:TRP:HB3	4:F:100:TYR:HB2	1.91	0.53
1:I:232:GLU:HB2	1:I:233:PHE:HA	1.91	0.53
3:U:91:LEU:CD2	4:T:100(B):PRO:HG3	2.39	0.52
4:C:121:VAL:HG12	4:C:209:LYS:HD2	1.92	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:I:211:GLU:OE2	5:I:501:NAG:H4	2.10	0.52
1:A:335:GLY:O	1:A:339:ASN:ND2	2.42	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:34:TRP:CH2	4:N:94:ARG:HG3	2.49	0.47
3:O:164:THR:HG21	4:N:164:HIS:HB3	1.96	0.47
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
1:B:232:GLU:HB2	1:B:233:PHE:HA	1.96	0.47
4:W:129:LYS:H	4:W:129:LYS:HD3	1.78	0.47
1:S:348:GLN:NE2	5:S:502:NAG:C8	2.76	0.47
1:M:461:ASN:O	1:M:463:ASN:N	2.47	0.47
3:D:108:ARG:NH1	3:D:111:ALA:HB2	2.30	0.47
1:S:344:GLN:HB3	5:S:502:NAG:O7	2.15	0.47
1:B:46:LYS:HD2	1:B:491:ILE:CD1	2.44	0.47
4:N:29:LEU:HD23	4:N:34:TRP:CZ2	2.50	0.47
1:M:232:GLU:CB	1:M:233:PHE:CA	2.92	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
3:K:37:GLN:O	3:K:45:LYS:N	2.47	0.46
1:A:350:ARG:O	1:A:352:TYR:N	2.45	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:N:34:TRP:CZ3	4:N:94:ARG:HB2	2.50	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: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
1:S:65:VAL:HB	1:S:115:SER:HB3	1.97	0.46
4:C:143:LYS:HG3	4:C:177:SER:HB2	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:S:348:GLN:HE21	5:S:502:NAG:C8	2.29	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
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:B:269:LYS:HG2	1:B:348:GLN:NE2	2.31	0.45
1:A:94:ASN:OD1	1:A:97:LYS:N	2.50	0.45

Continued on next page...

Continued from previous page...

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
3:K:36:TYR:HH	4:J:100(B):PRO:HB2	1.83	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
4:Q:129:LYS:HD3	4:Q:129:LYS:H	1.82	0.44
4:C:200:HIS:CE1	4:C:202:PRO:HB2	2.53	0.44
3:D:33:LEU:HD22	3:D:71:PHE:CG	2.53	0.44
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:B:327:ARG:NH2	1:B:422:GLN:OE1	2.49	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
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
1:A:77:THR:HB	1:A:78:ASP:CB	2.47	0.44
4:T:98:TRP:N	4:T:99:PRO:CA	2.79	0.44
3:K:118:PHE:HB3	4:J:124:LEU:HD22	1.99	0.44
4:C:12:LEU:HD11	4:C:18:LEU:HA	2.00	0.44
1:E:76:PRO:O	1:E:77:THR:OG1	2.24	0.44
4:F:33:TYR:HB2	4:F:95:ARG:HB2	2.00	0.44
1:S:269:LYS:HD3	5:S:502:NAG:C8	2.48	0.44
1:I:295:ASN:HD22	1:I:444:ARG:NH2	2.15	0.44
1:S:269:LYS:HD3	5:S:502:NAG:H83	1.99	0.43
3:G:126:LYS:HZ1	4:T:175:LEU:HD21	1.83	0.43
4:W:100(A):LEU:N	4:W:100(B):PRO:CD	2.81	0.43
3:D:58:VAL:HA	3:D:59:PRO:HD3	1.90	0.43
3:O:46:LEU:HD22	4:N:100(B):PRO:HB2	2.01	0.43
4:C:95:ARG:HB3	4:C:100(A):LEU:HD22	2.01	0.43
1:B:61:TYR:HD2	4:C:61:PRO:HA	1.83	0.43
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:HD23	4:T:178:LEU:C	2.40	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:A:278:THR:CG2	5:A:504:NAG:H62	2.50	0.42
1:S:61:TYR:CG	4:T:64:LYS:HD3	2.54	0.42
3:D:89:GLN:NE2	4:C:100(C):PHE:HE2	2.18	0.42
1:I:77:THR:HB	1:I:78:ASP:HB3	2.02	0.42
3:K:124:GLN:HG3	4:J:122:PHE:CE2	2.55	0.42
1:E:373:THR:O	1:E:374:HIS:CB	2.68	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:I:48:ALA:CB	1:I:49:ASN:HB2	2.50	0.41
1:B:212:PRO:CG	5:B:501:NAG:H2	2.50	0.41
3:K:13:ALA:HB3	3:K:104:LEU:HD11	2.02	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:I:298:ARG:NH2	1:I:441:GLY:O	2.52	0.41
3:X:116:PHE:CE2	4:W:132:SER:HB2	2.56	0.41
1:S:55:ALA:N	1:S:216:HIS:O	2.53	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:V:66:HIS:CE1	1:V:212:PRO:HA	2.55	0.41
1:I:232:GLU:CB	1:I:233:PHE:CA	2.96	0.41
4:T:52:LYS:HG3	4:T:54:ASN:H	1.85	0.41
4:C:201:LYS:N	4:C:202:PRO:CD	2.84	0.41
4:N:103:TRP:N	4:N:103:TRP:CD1	2.88	0.41
1:B:45:TRP:O	1:B:47:ASP:N	2.51	0.41
1:M:201:LEU:HD23	1:M:202:THR:N	2.35	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
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
3:L:49:TYR:HB3	4:H:100(B):PRO:HG3	2.03	0.41
1:A:77:THR:HB	1:A:78:ASP:CA	2.51	0.41
1:E:374:HIS:CD2	1:E:375:SER:N	2.89	0.41
1:M:96:TRP:CD2	1:M:275:GLU:HG3	2.56	0.41
3:D:149:LYS:N	3:D:193:ALA:O	2.43	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:76:PRO:O	1:S:77:THR:OG1	2.32	0.40
3:K:185:ASP:O	3:K:188:LYS:HG2	2.21	0.40
3:K:108:ARG:HH21	3:K:170:ASP:HB2	1.86	0.40
4:C:127:SER:OG	4:C:129:LYS:CE	2.69	0.40
3:D:158:ASN:O	3:D:179:LEU:HD12	2.21	0.40
3:D:142:ARG:O	3:D:142:ARG:HG2	2.20	0.40
1:V:55:ALA:N	1:V:216:HIS:O	2.53	0.40
1:P:55:ALA:N	1:P:216:HIS:O	2.54	0.40
3:R:33:LEU:HD22	3:R:71:PHE:CG	2.57	0.40
4:N:105:GLN:N	4:N:105:GLN:OE1	2.44	0.40
1:B:65:VAL:HB	1:B:115:SER:HB3	2.04	0.40
1:I:48:ALA:HB3	1:I:488:VAL:HG12	2.03	0.40
4:J:33:TYR:CZ	4:J:52:LYS:HD3	2.57	0.40
4:F:175:LEU:HD21	3:U:126:LYS:HZ1	1.85	0.40
1:E:325:ASP:OD1	1:E:326:ILE:N	2.54	0.40
4:C:159:LEU:HD21	4:C:182:VAL:HG21	2.03	0.40
1:B:232:GLU:HB3	1:B:233:PHE:HA	2.04	0.40
1:S:61:TYR:HD2	4:T:61:PRO:HA	1.87	0.40
3:D:33:LEU:HG	3:D:34:ALA:N	2.37	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%)	21	67
1	B	336/352 (96%)	301 (90%)	29 (9%)	6 (2%)	11	54
1	E	323/352 (92%)	290 (90%)	26 (8%)	7 (2%)	8	51
1	I	335/352 (95%)	285 (85%)	42 (12%)	8 (2%)	7	49
1	M	333/352 (95%)	298 (90%)	28 (8%)	7 (2%)	9	52
1	P	332/352 (94%)	295 (89%)	30 (9%)	7 (2%)	9	52
1	S	333/352 (95%)	293 (88%)	34 (10%)	6 (2%)	11	54
1	V	332/352 (94%)	299 (90%)	29 (9%)	4 (1%)	16	63
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%)	34	77
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%)	14	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	11	54
4	H	217/220 (99%)	204 (94%)	13 (6%)	0	100	100
4	J	217/220 (99%)	202 (93%)	11 (5%)	4 (2%)	11	54
4	N	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	14	59
4	Q	217/220 (99%)	203 (94%)	13 (6%)	1 (0%)	34	77
4	T	217/220 (99%)	203 (94%)	11 (5%)	3 (1%)	14	59
4	W	217/220 (99%)	198 (91%)	18 (8%)	1 (0%)	34	77
All	All	6243/6480 (96%)	5748 (92%)	427 (7%)	68 (1%)	17	64

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

Continued on next page...

Continued from previous page...

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/306 (96%)	287 (98%)	6 (2%)	63	87
1	B	299/306 (98%)	297 (99%)	2 (1%)	88	96
1	E	290/306 (95%)	288 (99%)	2 (1%)	88	96
1	I	298/306 (97%)	291 (98%)	7 (2%)	58	86
1	M	296/306 (97%)	293 (99%)	3 (1%)	82	93
1	P	295/306 (96%)	289 (98%)	6 (2%)	63	87
1	S	296/306 (97%)	290 (98%)	6 (2%)	63	87
1	V	296/306 (97%)	286 (97%)	10 (3%)	44	80
2	a	20/20 (100%)	19 (95%)	1 (5%)	30	70
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%)	40	77
3	G	183/183 (100%)	179 (98%)	4 (2%)	60	86
3	K	183/183 (100%)	182 (100%)	1 (0%)	92	97
3	L	183/183 (100%)	181 (99%)	2 (1%)	80	92
3	O	183/183 (100%)	180 (98%)	3 (2%)	70	90
3	R	183/183 (100%)	180 (98%)	3 (2%)	70	90
3	U	183/183 (100%)	178 (97%)	5 (3%)	52	83
3	X	183/183 (100%)	180 (98%)	3 (2%)	70	90
4	C	190/190 (100%)	180 (95%)	10 (5%)	28	69
4	F	190/190 (100%)	184 (97%)	6 (3%)	46	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	190/190 (100%)	186 (98%)	4 (2%)	61	87
4	J	190/190 (100%)	185 (97%)	5 (3%)	54	83
4	N	190/190 (100%)	179 (94%)	11 (6%)	25	66
4	Q	190/190 (100%)	187 (98%)	3 (2%)	70	90
4	T	190/190 (100%)	184 (97%)	6 (3%)	46	81
4	W	190/190 (100%)	183 (96%)	7 (4%)	41	77
All	All	5507/5592 (98%)	5384 (98%)	123 (2%)	60	86

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OAS	C	30	4	7,8,9	0.76	0	6,9,11	0.72	0

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	0.79	0	2,5,11	1.74	1 (50%)
4	OAS	H	30	4	7,8,9	0.73	0	6,9,11	0.82	0
4	OAS	J	30	4	4,5,9	0.79	0	2,5,11	1.73	1 (50%)
4	OAS	N	30	4	4,5,9	0.75	0	2,5,11	1.73	1 (50%)
4	OAS	Q	30	4	4,5,9	0.79	0	2,5,11	1.69	1 (50%)
4	OAS	T	30	4	7,8,9	0.76	0	6,9,11	0.71	0
4	OAS	W	30	4	7,8,9	0.76	0	6,9,11	0.63	0
2	DPR	a	21	2	6,7,8	0.60	0	7,8,10	1.22	1 (14%)
2	U2X	a	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	b	21	2	6,7,8	0.60	0	7,8,10	1.23	1 (14%)
2	U2X	b	23	2	19,20,21	2.30	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	e	21	2	6,7,8	0.60	0	7,8,10	1.22	1 (14%)
2	U2X	e	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	i	21	2	6,7,8	0.60	0	7,8,10	1.23	1 (14%)
2	U2X	i	23	2	19,20,21	2.30	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	m	21	2	6,7,8	0.62	0	7,8,10	1.23	1 (14%)
2	U2X	m	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.96	7 (31%)
2	DPR	p	21	2	6,7,8	0.60	0	7,8,10	1.22	1 (14%)
2	U2X	p	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	s	21	2	6,7,8	0.60	0	7,8,10	1.23	1 (14%)
2	U2X	s	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.97	7 (31%)
2	DPR	v	21	2	6,7,8	0.61	0	7,8,10	1.23	1 (14%)
2	U2X	v	23	2	19,20,21	2.29	5 (26%)	22,25,27	1.97	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	C	30	4	-	0/5/7/9	0/0/0/0
4	OAS	F	30	4	-	0/2/4/9	0/0/0/0
4	OAS	H	30	4	-	1/5/7/9	0/0/0/0
4	OAS	J	30	4	-	0/2/4/9	0/0/0/0
4	OAS	N	30	4	-	0/2/4/9	0/0/0/0
4	OAS	Q	30	4	-	0/2/4/9	0/0/0/0
4	OAS	T	30	4	-	0/5/7/9	0/0/0/0
4	OAS	W	30	4	-	0/5/7/9	0/0/0/0

Continued on next page...

Continued from previous page...

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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	23	U2X	CB-CA	-2.12	1.49	1.53
2	p	23	U2X	CB-CA	-2.12	1.49	1.53
2	b	23	U2X	CB-CA	-2.11	1.49	1.53
2	a	23	U2X	CB-CA	-2.11	1.49	1.53
2	i	23	U2X	CB-CA	-2.10	1.49	1.53
2	m	23	U2X	CB-CA	-2.10	1.49	1.53
2	s	23	U2X	CB-CA	-2.10	1.49	1.53
2	v	23	U2X	CB-CA	-2.09	1.49	1.53
2	e	23	U2X	C4-C3	2.30	1.58	1.52
2	i	23	U2X	C4-C3	2.31	1.58	1.52
2	b	23	U2X	C4-C3	2.31	1.58	1.52
2	v	23	U2X	C4-C3	2.31	1.58	1.52
2	a	23	U2X	C4-C3	2.32	1.58	1.52
2	m	23	U2X	C4-C3	2.32	1.58	1.52
2	s	23	U2X	C4-C3	2.32	1.58	1.52
2	p	23	U2X	C4-C3	2.33	1.58	1.52
2	i	23	U2X	CE1-CZ	2.54	1.43	1.38
2	p	23	U2X	CE1-CZ	2.54	1.43	1.38
2	s	23	U2X	CE1-CZ	2.54	1.43	1.38
2	a	23	U2X	CE1-CZ	2.54	1.43	1.38
2	v	23	U2X	CE1-CZ	2.54	1.43	1.38
2	b	23	U2X	CE1-CZ	2.55	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	e	23	U2X	CE1-CZ	2.56	1.43	1.38
2	m	23	U2X	CE1-CZ	2.57	1.43	1.38
2	v	23	U2X	CE1-CD1	4.18	1.46	1.38
2	s	23	U2X	CE1-CD1	4.20	1.46	1.38
2	m	23	U2X	CE1-CD1	4.21	1.46	1.38
2	a	23	U2X	CE1-CD1	4.22	1.46	1.38
2	b	23	U2X	CE1-CD1	4.22	1.46	1.38
2	e	23	U2X	CE1-CD1	4.23	1.46	1.38
2	p	23	U2X	CE1-CD1	4.24	1.46	1.38
2	i	23	U2X	CE1-CD1	4.24	1.46	1.38
2	e	23	U2X	CE2-CD2	7.21	1.51	1.38
2	p	23	U2X	CE2-CD2	7.22	1.51	1.38
2	m	23	U2X	CE2-CD2	7.23	1.51	1.38
2	a	23	U2X	CE2-CD2	7.24	1.51	1.38
2	i	23	U2X	CE2-CD2	7.26	1.51	1.38
2	s	23	U2X	CE2-CD2	7.26	1.51	1.38
2	v	23	U2X	CE2-CD2	7.27	1.51	1.38
2	b	23	U2X	CE2-CD2	7.29	1.51	1.38

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	23	U2X	C1-C2-C3	-3.29	106.92	112.22
2	i	23	U2X	C1-C2-C3	-3.27	106.94	112.22
2	e	23	U2X	C1-C2-C3	-3.26	106.95	112.22
2	p	23	U2X	C1-C2-C3	-3.26	106.96	112.22
2	a	23	U2X	C1-C2-C3	-3.26	106.96	112.22
2	v	23	U2X	C1-C2-C3	-3.26	106.97	112.22
2	s	23	U2X	C1-C2-C3	-3.26	106.97	112.22
2	m	23	U2X	C1-C2-C3	-3.25	106.98	112.22
2	v	23	U2X	C5-C4-C3	-2.75	107.78	112.22
2	a	23	U2X	C5-C4-C3	-2.74	107.80	112.22
2	p	23	U2X	C5-C4-C3	-2.74	107.80	112.22
2	b	23	U2X	C5-C4-C3	-2.74	107.80	112.22
2	m	23	U2X	C5-C4-C3	-2.74	107.81	112.22
2	e	23	U2X	C5-C4-C3	-2.73	107.82	112.22
2	s	23	U2X	C5-C4-C3	-2.73	107.82	112.22
2	i	23	U2X	C5-C4-C3	-2.72	107.83	112.22
4	F	30	OAS	OG-CB-CA	-2.41	105.61	111.08
4	Q	30	OAS	OG-CB-CA	-2.36	105.73	111.08
4	N	30	OAS	OG-CB-CA	-2.34	105.78	111.08
4	J	30	OAS	OG-CB-CA	-2.33	105.80	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	m	21	DPR	O-C-CA	-2.11	119.86	125.44
2	e	21	DPR	O-C-CA	-2.11	119.86	125.44
2	a	21	DPR	O-C-CA	-2.11	119.87	125.44
2	b	21	DPR	O-C-CA	-2.11	119.88	125.44
2	s	21	DPR	O-C-CA	-2.10	119.88	125.44
2	i	21	DPR	O-C-CA	-2.10	119.89	125.44
2	v	21	DPR	O-C-CA	-2.10	119.91	125.44
2	p	21	DPR	O-C-CA	-2.09	119.91	125.44
2	v	23	U2X	CD2-CG-CD1	2.14	121.56	118.13
2	e	23	U2X	CD2-CG-CD1	2.15	121.58	118.13
2	m	23	U2X	CD2-CG-CD1	2.15	121.58	118.13
2	a	23	U2X	CD2-CG-CD1	2.16	121.59	118.13
2	p	23	U2X	CD2-CG-CD1	2.17	121.60	118.13
2	i	23	U2X	CD2-CG-CD1	2.18	121.62	118.13
2	s	23	U2X	CD2-CG-CD1	2.19	121.63	118.13
2	b	23	U2X	CD2-CG-CD1	2.19	121.64	118.13
2	p	23	U2X	CG-CB-CA	2.58	120.02	114.21
2	s	23	U2X	CG-CB-CA	2.58	120.03	114.21
2	a	23	U2X	CG-CB-CA	2.59	120.05	114.21
2	m	23	U2X	CG-CB-CA	2.59	120.05	114.21
2	b	23	U2X	CG-CB-CA	2.59	120.06	114.21
2	v	23	U2X	CG-CB-CA	2.60	120.07	114.21
2	e	23	U2X	CG-CB-CA	2.60	120.07	114.21
2	i	23	U2X	CG-CB-CA	2.60	120.07	114.21
2	e	23	U2X	OH-C7-C3	2.72	114.25	107.97
2	v	23	U2X	OH-C7-C3	2.72	114.25	107.97
2	i	23	U2X	OH-C7-C3	2.73	114.25	107.97
2	s	23	U2X	OH-C7-C3	2.73	114.26	107.97
2	a	23	U2X	OH-C7-C3	2.73	114.27	107.97
2	m	23	U2X	OH-C7-C3	2.74	114.29	107.97
2	p	23	U2X	OH-C7-C3	2.75	114.30	107.97
2	b	23	U2X	OH-C7-C3	2.75	114.31	107.97
2	p	23	U2X	C4-C3-C7	3.25	118.32	111.47
2	a	23	U2X	C4-C3-C7	3.25	118.33	111.47
2	m	23	U2X	C4-C3-C7	3.26	118.34	111.47
2	v	23	U2X	C4-C3-C7	3.26	118.34	111.47
2	b	23	U2X	C4-C3-C7	3.26	118.34	111.47
2	e	23	U2X	C4-C3-C7	3.26	118.35	111.47
2	i	23	U2X	C4-C3-C7	3.27	118.36	111.47
2	s	23	U2X	C4-C3-C7	3.27	118.37	111.47
2	b	23	U2X	C2-C3-C7	4.80	121.59	111.47
2	s	23	U2X	C2-C3-C7	4.82	121.63	111.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	a	23	U2X	C2-C3-C7	4.82	121.63	111.47
2	v	23	U2X	C2-C3-C7	4.82	121.63	111.47
2	i	23	U2X	C2-C3-C7	4.82	121.64	111.47
2	p	23	U2X	C2-C3-C7	4.83	121.65	111.47
2	e	23	U2X	C2-C3-C7	4.83	121.66	111.47
2	m	23	U2X	C2-C3-C7	4.83	121.66	111.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	501	1	14,14,15	0.44	0	15,19,21	0.26	0
5	NAG	A	502	1	14,14,15	0.26	0	15,19,21	0.33	0
5	NAG	A	503	1	14,14,15	0.20	0	15,19,21	0.35	0
5	NAG	A	504	1	14,14,15	0.18	0	15,19,21	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	501	1	14,14,15	0.22	0	15,19,21	0.34	0
5	NAG	B	502	1	14,14,15	0.34	0	15,19,21	1.30	1 (6%)
5	NAG	E	501	1	14,14,15	0.27	0	15,19,21	0.31	0
5	NAG	E	502	1	14,14,15	0.25	0	15,19,21	0.35	0
5	NAG	I	501	1	14,14,15	0.27	0	15,19,21	0.46	0
5	NAG	I	502	1	14,14,15	0.35	0	15,19,21	0.40	0
5	NAG	I	503	1	14,14,15	0.22	0	15,19,21	0.32	0
5	NAG	I	504	1	14,14,15	0.50	0	15,19,21	0.20	0
5	NAG	M	501	1	14,14,15	0.26	0	15,19,21	0.39	0
5	NAG	P	501	1	14,14,15	0.23	0	15,19,21	0.21	0
5	NAG	P	502	1	14,14,15	0.31	0	15,19,21	0.46	0
5	NAG	S	501	1	14,14,15	0.23	0	15,19,21	0.30	0
5	NAG	S	502	1	14,14,15	0.49	0	15,19,21	0.58	0
5	NAG	S	503	1	14,14,15	0.26	0	15,19,21	0.28	0
5	NAG	V	501	1	14,14,15	0.33	0	15,19,21	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	501	1	-	0/6/23/26	0/1/1/1
5	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	NAG	A	504	1	-	0/6/23/26	0/1/1/1
5	NAG	B	501	1	-	0/6/23/26	0/1/1/1
5	NAG	B	502	1	-	0/6/23/26	0/1/1/1
5	NAG	E	501	1	-	0/6/23/26	0/1/1/1
5	NAG	E	502	1	-	0/6/23/26	0/1/1/1
5	NAG	I	501	1	-	0/6/23/26	0/1/1/1
5	NAG	I	502	1	-	0/6/23/26	0/1/1/1
5	NAG	I	503	1	-	0/6/23/26	0/1/1/1
5	NAG	I	504	1	-	0/6/23/26	0/1/1/1
5	NAG	M	501	1	-	0/6/23/26	0/1/1/1
5	NAG	P	501	1	-	0/6/23/26	0/1/1/1
5	NAG	P	502	1	-	0/6/23/26	0/1/1/1
5	NAG	S	501	1	-	0/6/23/26	0/1/1/1
5	NAG	S	502	1	-	0/6/23/26	0/1/1/1
5	NAG	S	503	1	-	0/6/23/26	0/1/1/1
5	NAG	V	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	502	NAG	C1-O5-C5	4.54	118.01	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 49 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/352 (94%)	0.56	31 (9%) 11 9	119, 153, 203, 222	0
1	B	342/352 (97%)	0.60	42 (12%) 5 6	105, 174, 268, 299	0
1	E	329/352 (93%)	0.70	48 (14%) 3 3	141, 205, 256, 283	0
1	I	341/352 (96%)	0.41	27 (7%) 15 12	120, 166, 210, 232	0
1	M	339/352 (96%)	0.59	41 (12%) 6 6	122, 188, 245, 262	0
1	P	338/352 (96%)	0.56	33 (9%) 10 9	104, 170, 241, 263	0
1	S	339/352 (96%)	0.56	26 (7%) 16 13	123, 177, 252, 283	0
1	V	338/352 (96%)	0.60	31 (9%) 11 10	122, 180, 263, 301	0
2	a	24/28 (85%)	0.39	2 (8%) 14 12	141, 188, 204, 208	0
2	b	24/28 (85%)	0.32	1 (4%) 40 32	161, 195, 225, 229	0
2	e	24/28 (85%)	0.18	1 (4%) 40 32	171, 198, 220, 223	0
2	i	24/28 (85%)	0.14	1 (4%) 40 32	140, 189, 200, 204	0
2	m	24/28 (85%)	0.40	2 (8%) 14 12	171, 209, 228, 233	0
2	p	24/28 (85%)	0.40	1 (4%) 40 32	118, 160, 181, 188	0
2	s	24/28 (85%)	0.36	2 (8%) 14 12	149, 202, 226, 231	0
2	v	24/28 (85%)	0.32	4 (16%) 2 2	170, 213, 220, 221	0
3	D	210/210 (100%)	1.31	52 (24%) 1 1	106, 227, 332, 347	0
3	G	210/210 (100%)	1.36	52 (24%) 1 1	172, 252, 328, 358	0
3	K	210/210 (100%)	2.80	84 (40%) 0 1	210, 340, 366, 371	0
3	L	210/210 (100%)	0.63	30 (14%) 4 3	146, 230, 276, 302	0
3	O	210/210 (100%)	1.25	55 (26%) 1 1	193, 256, 292, 314	0
3	R	210/210 (100%)	1.31	50 (23%) 1 1	181, 250, 340, 377	0
3	U	210/210 (100%)	0.75	32 (15%) 3 3	117, 227, 317, 334	0
3	X	210/210 (100%)	1.47	68 (32%) 1 1	185, 248, 303, 317	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
4	C	219/220 (99%)	1.07	51 (23%)	1 1	102, 188, 337, 353	0
4	F	219/220 (99%)	1.01	52 (23%)	1 1	189, 240, 283, 314	0
4	H	219/220 (99%)	0.68	41 (18%)	2 2	144, 198, 268, 280	0
4	J	219/220 (99%)	1.84	77 (35%)	0 1	205, 303, 380, 398	0
4	N	219/220 (99%)	1.36	58 (26%)	1 1	189, 240, 282, 300	0
4	Q	219/220 (99%)	0.92	47 (21%)	1 1	179, 241, 285, 310	0
4	T	219/220 (99%)	1.12	47 (21%)	1 1	125, 212, 311, 338	0
4	W	219/220 (99%)	1.19	61 (27%)	1 1	170, 232, 271, 292	0
All	All	6323/6480 (97%)	0.93	1150 (18%)	2 2	102, 208, 323, 398	0

All (1150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	197	THR	28.7
3	K	144	ALA	26.7
3	K	136	LEU	26.2
4	J	179	SER	24.0
3	K	115	VAL	22.3
3	R	149	LYS	17.3
3	D	193	ALA	17.2
4	J	11	LEU	16.2
3	K	175	LEU	15.8
3	K	34	ALA	15.2
3	K	145	LYS	14.9
3	U	181	LEU	14.3
3	G	150	VAL	14.2
4	T	211	VAL	13.8
3	R	150	VAL	13.3
3	K	177	SER	13.2
3	G	181	LEU	13.2
4	J	109	VAL	13.1
1	V	459	GLY	13.0
4	F	179	SER	12.9
3	K	21	ILE	12.8
4	C	180	SER	12.6
3	K	73	LEU	12.6
4	N	184	VAL	12.6
3	K	19	VAL	12.5
1	P	406	THR	12.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	209	PHE	12.2
4	T	161	SER	11.7
4	F	69	ILE	11.7
3	K	135	LEU	11.7
4	J	147	PRO	11.5
1	M	285	ILE	11.4
1	E	453	ILE	11.3
3	G	132	VAL	11.3
1	A	359	ILE	10.8
3	D	181	LEU	10.6
3	O	11	VAL	10.6
3	X	132	VAL	10.3
3	O	104	LEU	10.2
3	D	150	VAL	10.0
3	K	116	PHE	10.0
4	T	126	PRO	10.0
3	G	149	LYS	9.9
3	K	134	CYS	9.8
4	W	211	VAL	9.8
4	J	12	LEU	9.6
3	G	131	SER	9.6
3	K	161	GLU	9.6
3	G	116	PHE	9.5
3	O	192	TYR	9.4
3	D	135	LEU	9.4
1	V	359	ILE	9.3
3	G	25	ALA	9.3
1	M	359	ILE	9.3
3	G	192	TYR	9.3
1	S	359	ILE	9.1
4	N	129	LYS	9.1
4	W	119	PRO	9.0
4	N	114	ALA	9.0
3	X	131	SER	8.9
4	F	180	SER	8.9
3	O	131	SER	8.9
3	K	20	THR	8.9
3	X	186	TYR	8.8
4	F	129	LYS	8.8
4	C	211	VAL	8.8
4	Q	140	CYS	8.8
1	B	408	SER	8.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	111	VAL	8.8
3	G	133	VAL	8.7
1	E	286	VAL	8.7
3	O	51	ALA	8.6
3	L	181	LEU	8.6
3	K	204	PRO	8.5
3	R	116	PHE	8.5
4	N	112	SER	8.5
1	M	286	VAL	8.4
3	D	144	ALA	8.4
3	D	134	CYS	8.4
3	D	192	TYR	8.4
3	K	14	SER	8.3
1	E	452	LEU	8.2
4	J	69	ILE	8.1
4	C	184	VAL	8.1
3	R	181	LEU	8.0
1	E	284	ILE	7.9
4	W	69	ILE	7.9
4	J	178	LEU	7.8
3	G	47	VAL	7.8
3	D	152	ASN	7.8
4	W	112	SER	7.8
1	E	283	ASN	7.8
4	J	9	ALA	7.8
4	J	180	SER	7.8
3	X	194	CYS	7.7
1	E	285	ILE	7.7
3	R	134	CYS	7.7
3	R	133	VAL	7.6
3	K	203	SER	7.6
3	X	117	ILE	7.6
3	X	133	VAL	7.5
3	K	196	VAL	7.5
1	S	338	TRP	7.5
3	X	193	ALA	7.4
4	C	140	CYS	7.4
3	K	133	VAL	7.2
3	X	62	PHE	7.2
4	W	29	LEU	7.2
3	R	193	ALA	7.2
4	N	130	SER	7.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	N	179	SER	7.2
4	C	138	LEU	7.2
4	N	18	LEU	7.1
3	K	82	ASP	7.1
3	K	33	LEU	7.1
3	K	147	GLN	7.0
4	F	111	VAL	7.0
3	K	180	THR	6.9
3	U	209	PHE	6.9
3	G	193	ALA	6.9
1	P	453	ILE	6.9
4	J	110	THR	6.9
3	D	149	LYS	6.9
3	R	180	THR	6.9
4	N	160	THR	6.8
4	J	33	TYR	6.8
3	U	17	ASP	6.8
4	N	111	VAL	6.8
4	C	185	PRO	6.7
3	K	46	LEU	6.7
4	W	18	LEU	6.7
1	E	258	GLN	6.7
3	O	142	ARG	6.7
1	S	286	VAL	6.7
3	O	50	ALA	6.7
3	X	181	LEU	6.7
3	D	205	VAL	6.6
3	X	207	LYS	6.6
3	G	191	VAL	6.6
3	R	86	TYR	6.6
4	F	48	ILE	6.5
3	K	47	VAL	6.5
4	J	18	LEU	6.5
4	N	82	LEU	6.5
3	K	113	PRO	6.5
4	F	93	ALA	6.5
4	J	194	TYR	6.5
1	B	453	ILE	6.5
4	F	141	LEU	6.4
4	H	54	ASN	6.4
3	D	25	ALA	6.4
1	V	93	PHE	6.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	C	183	THR	6.4
4	Q	29	LEU	6.4
4	F	29	LEU	6.4
3	O	12	SER	6.4
3	X	76	SER	6.4
1	P	284	ILE	6.4
4	Q	179	SER	6.3
1	M	259	LEU	6.3
4	W	67	VAL	6.3
3	K	181	LEU	6.3
4	W	160	THR	6.3
3	U	113	PRO	6.3
4	F	142	VAL	6.3
3	G	12	SER	6.3
4	J	35	SER	6.2
3	G	87	TYR	6.2
4	C	181	VAL	6.2
4	Q	27	GLU	6.2
4	Q	38	ARG	6.2
1	M	473	GLY	6.2
1	A	286	VAL	6.2
4	T	110	THR	6.2
1	A	284	ILE	6.1
1	E	454	LEU	6.1
4	C	139	GLY	6.1
1	V	338	TRP	6.1
4	J	166	PHE	6.1
3	K	205	VAL	6.1
4	W	126	PRO	6.1
3	K	174	SER	6.1
3	R	201	LEU	6.0
3	U	151	ASP	6.0
4	J	123	PRO	6.0
4	J	130	SER	6.0
4	F	181	VAL	6.0
1	A	452	LEU	6.0
1	M	452	LEU	6.0
1	M	284	ILE	6.0
3	L	192	TYR	6.0
3	K	165	GLU	6.0
1	S	259	LEU	6.0
3	K	13	ALA	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	146	VAL	6.0
4	F	67	VAL	6.0
4	J	129	LYS	6.0
4	W	121	VAL	5.9
4	J	164	HIS	5.9
3	K	25	ALA	5.9
4	C	11	LEU	5.9
4	H	189	LEU	5.9
1	I	286	VAL	5.9
3	L	115	VAL	5.9
4	C	18	LEU	5.8
3	X	168	SER	5.8
3	X	41	GLY	5.8
1	B	359	ILE	5.8
3	L	116	PHE	5.8
4	N	126	PRO	5.8
4	Q	37	VAL	5.8
4	N	110	THR	5.8
3	R	135	LEU	5.8
1	V	452	LEU	5.7
3	O	29	ILE	5.7
3	G	11	VAL	5.7
3	G	151	ASP	5.7
1	E	349	LEU	5.7
3	O	86	TYR	5.7
1	M	349	LEU	5.7
1	P	452	LEU	5.7
4	C	194	TYR	5.7
3	O	4	MET	5.7
3	D	201	LEU	5.7
3	X	29	ILE	5.7
3	X	36	TYR	5.7
3	G	32	TYR	5.7
4	H	150	VAL	5.7
3	R	205	VAL	5.7
3	O	54	LEU	5.6
3	G	13	ALA	5.6
3	K	154	LEU	5.6
3	G	196	VAL	5.6
4	J	137	ALA	5.6
2	a	27	VAL	5.6
1	B	259	LEU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	W	37	VAL	5.5
1	M	338	TRP	5.5
4	J	71	LEU	5.5
3	D	131	SER	5.5
3	X	192	TYR	5.5
4	H	138	LEU	5.5
3	G	118	PHE	5.5
1	S	414	ILE	5.5
1	B	338	TRP	5.5
4	J	34	TRP	5.5
3	X	148	TRP	5.4
1	I	287	GLN	5.4
1	A	290	GLU	5.4
3	K	87	TYR	5.4
4	N	136	ALA	5.4
4	Q	35	SER	5.4
3	R	25	ALA	5.4
4	J	59	TYR	5.4
4	J	165	THR	5.4
3	R	196	VAL	5.3
1	V	259	LEU	5.3
4	C	35	SER	5.3
4	T	109	VAL	5.3
4	N	198	VAL	5.3
3	G	86	TYR	5.3
4	T	9	ALA	5.3
4	F	150	VAL	5.3
1	P	359	ILE	5.3
4	W	110	THR	5.3
3	D	180	THR	5.3
3	L	133	VAL	5.3
3	O	132	VAL	5.3
4	H	90	TYR	5.3
1	I	359	ILE	5.2
4	N	69	ILE	5.2
1	M	77	THR	5.2
4	W	111	VAL	5.2
4	W	161	SER	5.2
4	T	186	SER	5.2
1	B	258	GLN	5.2
4	T	29	LEU	5.2
1	B	242	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	15	VAL	5.1
4	N	107	THR	5.1
3	K	155	GLN	5.1
1	M	361	PHE	5.1
3	K	194	CYS	5.1
4	T	18	LEU	5.0
4	C	123	PRO	5.0
1	E	359	ILE	5.0
3	K	150	VAL	5.0
3	O	41	GLY	5.0
3	K	114	SER	5.0
4	J	210	LYS	5.0
1	M	488	VAL	5.0
4	T	129	LYS	5.0
3	L	135	LEU	4.9
1	V	253	PRO	4.9
4	J	149	PRO	4.9
3	L	35	TRP	4.9
4	C	82	LEU	4.9
4	J	148	GLU	4.9
1	V	409	ILE	4.9
3	D	153	ALA	4.9
4	H	11	LEU	4.9
4	F	109	VAL	4.9
1	V	272	ILE	4.9
4	W	96	SER	4.8
3	D	198	HIS	4.8
3	U	142	ARG	4.8
3	R	151	ASP	4.8
4	C	122	PHE	4.8
3	R	207	LYS	4.8
1	M	50	THR	4.8
4	W	132	SER	4.8
3	O	210	ASN	4.8
4	N	71	LEU	4.8
4	T	209	LYS	4.8
3	O	144	ALA	4.8
1	A	285	ILE	4.8
3	K	62	PHE	4.7
1	I	285	ILE	4.7
1	I	407	ALA	4.7
3	K	206	THR	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	J	87	THR	4.7
4	T	82	LEU	4.7
4	Q	36	TRP	4.7
4	T	25	TYR	4.7
1	P	338	TRP	4.7
1	P	454	LEU	4.7
3	R	62	PHE	4.7
3	D	136	LEU	4.7
3	U	193	ALA	4.7
3	D	147	GLN	4.6
1	A	453	ILE	4.6
3	R	47	VAL	4.6
4	W	71	LEU	4.6
2	p	17	GLY	4.6
3	D	196	VAL	4.6
1	B	407	ALA	4.6
1	V	453	ILE	4.6
3	R	87	TYR	4.6
4	T	34	TRP	4.6
4	J	27	GLU	4.6
3	K	211	ARG	4.6
3	X	51	ALA	4.6
4	J	29	LEU	4.6
1	P	58	ALA	4.5
1	A	492	GLU	4.5
3	O	103	LYS	4.5
3	O	130	ALA	4.5
4	F	35	SER	4.5
3	O	118	PHE	4.5
4	T	214	LYS	4.5
4	H	110	THR	4.5
3	R	19	VAL	4.5
4	J	8	GLY	4.5
1	P	471	GLY	4.5
4	W	213	PRO	4.5
4	J	108	LEU	4.5
4	T	56	SER	4.5
3	R	132	VAL	4.5
4	H	10	GLY	4.5
4	C	186	SER	4.5
3	D	115	VAL	4.5
1	V	284	ILE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	473	GLY	4.4
4	J	86	ASP	4.4
3	R	24	ARG	4.4
4	J	195	ILE	4.4
3	U	192	TYR	4.4
4	C	108	LEU	4.4
4	W	82	LEU	4.4
3	R	152	ASN	4.4
3	U	150	VAL	4.4
4	F	100(C)	PHE	4.4
1	M	260	LEU	4.3
3	G	33	LEU	4.3
1	V	258	GLN	4.3
4	Q	110	THR	4.3
3	L	144	ALA	4.3
3	K	149	LYS	4.3
3	G	134	CYS	4.3
3	O	62	PHE	4.3
4	N	11	LEU	4.3
3	D	86	TYR	4.3
1	B	86	MET	4.3
3	L	78	LEU	4.3
2	s	27	VAL	4.3
1	V	390	LEU	4.3
3	L	134	CYS	4.3
4	N	185	PRO	4.3
3	G	117	ILE	4.3
1	B	281	VAL	4.2
4	W	207	VAL	4.2
1	A	287	GLN	4.2
3	G	161	GLU	4.2
4	H	109	VAL	4.2
4	F	27	GLU	4.2
4	W	12	LEU	4.2
1	E	242	VAL	4.2
3	G	135	LEU	4.2
4	Q	80	LEU	4.2
1	E	357	ASN	4.2
4	T	10	GLY	4.2
1	M	254	VAL	4.2
4	H	17	THR	4.2
3	O	10	PHE	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	82	GLN	4.1
4	H	18	LEU	4.1
1	B	452	LEU	4.1
3	L	47	VAL	4.1
3	K	143	GLU	4.1
3	X	129	THR	4.1
1	A	338	TRP	4.1
1	A	483	LEU	4.1
4	J	189	LEU	4.1
1	E	259	LEU	4.1
4	W	122	PHE	4.1
4	W	141	LEU	4.1
1	I	338	TRP	4.0
1	S	285	ILE	4.0
4	H	80	LEU	4.0
4	Q	69	ILE	4.0
1	I	60	ALA	4.0
4	J	93	ALA	4.0
1	I	50	THR	4.0
3	X	115	VAL	4.0
4	H	213	PRO	4.0
1	S	452	LEU	4.0
1	P	283	ASN	4.0
3	R	194	CYS	4.0
1	P	349	LEU	4.0
4	H	67	VAL	4.0
3	K	148	TRP	4.0
1	A	361	PHE	4.0
4	C	137	ALA	3.9
4	T	11	LEU	3.9
1	B	45	TRP	3.9
3	L	209	PHE	3.9
3	G	24	ARG	3.9
3	R	17	ASP	3.9
3	R	153	ALA	3.9
3	U	191	VAL	3.9
4	J	190	GLY	3.9
1	E	301	ASN	3.9
3	L	118	PHE	3.9
4	C	126	PRO	3.9
1	P	258	GLN	3.9
3	L	29	ILE	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	G	62	PHE	3.9
4	Q	91	PHE	3.9
4	J	181	VAL	3.9
1	M	453	ILE	3.9
4	J	82	LEU	3.9
3	X	11	VAL	3.9
1	B	468	PHE	3.9
4	T	100(C)	PHE	3.9
4	J	73	MET	3.9
4	C	182	VAL	3.9
4	N	4	LEU	3.9
4	Q	126	PRO	3.9
1	S	453	ILE	3.9
3	O	35	TRP	3.9
1	B	420	ILE	3.8
3	U	180	THR	3.8
4	N	146	PHE	3.8
1	A	468	PHE	3.8
1	A	349	LEU	3.8
3	G	179	LEU	3.8
3	U	196	VAL	3.8
3	U	161	GLU	3.8
4	N	127	SER	3.8
1	B	333	VAL	3.8
1	I	284	ILE	3.8
1	S	58	ALA	3.8
3	L	33	LEU	3.8
4	F	130	SER	3.8
4	T	189	LEU	3.8
4	H	137	ALA	3.8
3	D	33	LEU	3.8
4	C	20	LEU	3.8
3	R	92	ILE	3.7
3	O	1	ASP	3.7
4	N	207	VAL	3.7
4	J	10	GLY	3.7
4	J	102	PRO	3.7
3	K	132	VAL	3.7
3	X	77	SER	3.7
4	N	12	LEU	3.7
4	H	108	LEU	3.7
4	N	152	VAL	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	W	124	LEU	3.7
4	Q	11	LEU	3.7
1	V	349	LEU	3.7
3	R	128	GLY	3.7
3	K	163	VAL	3.6
3	O	194	CYS	3.6
1	A	451	GLY	3.6
3	O	191	VAL	3.6
3	K	83	PHE	3.6
1	M	217	TYR	3.6
4	C	38	ARG	3.6
3	D	116	PHE	3.6
4	F	110	THR	3.6
4	J	167	PRO	3.6
4	N	142	VAL	3.6
3	X	104	LEU	3.6
3	R	147	GLN	3.6
2	v	27	VAL	3.6
3	K	190	LYS	3.6
4	N	67	VAL	3.6
3	L	149	LYS	3.6
4	W	80	LEU	3.6
1	B	339	ASN	3.6
1	M	261	LEU	3.6
3	K	193	ALA	3.6
3	R	161	GLU	3.6
4	J	45	LEU	3.6
3	D	82	ASP	3.5
1	P	100	MET	3.5
4	F	205	THR	3.5
1	M	272	ILE	3.5
3	D	133	VAL	3.5
3	K	162	SER	3.5
4	N	14	PRO	3.5
3	O	84	ALA	3.5
1	S	381	GLU	3.5
3	L	130	ALA	3.5
3	U	118	PHE	3.5
4	F	34	TRP	3.5
1	V	285	ILE	3.5
1	A	288	LEU	3.5
3	X	102	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	O	21	ILE	3.5
1	V	374	HIS	3.5
4	Q	20	LEU	3.5
4	W	125	ALA	3.5
4	Q	214	LYS	3.5
4	W	129	LYS	3.5
1	B	284	ILE	3.5
1	M	346	VAL	3.5
4	W	113	SER	3.5
4	F	91	PHE	3.5
3	K	110	VAL	3.5
4	T	59	TYR	3.5
1	P	213	ILE	3.4
3	D	124	GLN	3.4
3	D	137	ASN	3.4
1	I	454	LEU	3.4
2	m	26	CYS	3.4
4	W	140	CYS	3.4
3	R	136	LEU	3.4
3	O	196	VAL	3.4
1	P	285	ILE	3.4
3	D	203	SER	3.4
1	E	282	LYS	3.4
1	E	338	TRP	3.4
4	H	198	VAL	3.4
3	K	22	THR	3.4
4	J	115	SER	3.4
3	X	33	LEU	3.4
1	S	468	PHE	3.4
1	P	322	SER	3.4
3	X	47	VAL	3.4
4	F	18	LEU	3.3
1	S	287	GLN	3.3
4	N	140	CYS	3.3
4	F	68	THR	3.3
4	F	87	THR	3.3
1	B	405	GLY	3.3
4	C	9	ALA	3.3
4	W	210	LYS	3.3
3	D	204	PRO	3.3
3	G	144	ALA	3.3
4	W	114	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	194	TYR	3.3
1	I	335	GLY	3.3
3	U	78	LEU	3.3
3	X	178	THR	3.3
3	G	210	ASN	3.3
4	J	98	TRP	3.3
1	S	342	LEU	3.3
1	V	408	SER	3.3
3	D	114	SER	3.3
4	N	131	THR	3.3
4	W	154	TRP	3.3
4	F	178	LEU	3.3
1	P	470	PRO	3.2
4	W	91	PHE	3.2
4	H	140	CYS	3.2
4	J	193	THR	3.2
4	Q	71	LEU	3.2
3	G	141	PRO	3.2
3	R	1	ASP	3.2
4	T	50	GLU	3.2
4	N	91	PHE	3.2
1	E	83	GLU	3.2
1	B	294	ILE	3.2
4	C	135	THR	3.2
3	K	126	LYS	3.2
3	O	122	ASP	3.2
1	I	406	THR	3.2
3	X	130	ALA	3.2
4	C	19	SER	3.2
3	R	115	VAL	3.2
4	N	87	THR	3.2
3	R	46	LEU	3.2
3	X	60	SER	3.2
3	O	133	VAL	3.2
3	O	13	ALA	3.2
4	F	213	PRO	3.2
4	T	137	ALA	3.2
3	K	86	TYR	3.2
4	J	92	CYS	3.2
1	A	342	LEU	3.2
1	P	468	PHE	3.2
4	Q	98	TRP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	W	34	TRP	3.2
4	W	212	GLU	3.2
1	E	361	PHE	3.2
4	C	170	LEU	3.2
3	K	17	ASP	3.1
3	L	201	LEU	3.1
1	E	56	SER	3.1
3	R	117	ILE	3.1
4	H	126	PRO	3.1
4	W	109	VAL	3.1
3	D	117	ILE	3.1
4	C	124	LEU	3.1
1	E	383	PHE	3.1
3	R	183	LYS	3.1
4	T	154	TRP	3.1
1	V	60	ALA	3.1
4	T	150	VAL	3.1
4	H	71	LEU	3.1
3	X	19	VAL	3.1
4	N	161	SER	3.1
1	M	451	GLY	3.1
1	S	49	ASN	3.1
3	X	167	ASP	3.1
4	W	48	ILE	3.1
1	P	49	ASN	3.1
4	C	207	VAL	3.1
1	E	342	LEU	3.1
3	G	2	ILE	3.0
3	X	185	ASP	3.0
4	J	158	ALA	3.0
1	E	49	ASN	3.0
3	X	187	GLU	3.0
1	V	414	ILE	3.0
3	K	10	PHE	3.0
4	H	100(C)	PHE	3.0
4	W	100(C)	PHE	3.0
1	V	410	GLU	3.0
3	O	102	THR	3.0
3	K	187	GLU	3.0
3	K	153	ALA	3.0
4	F	115	SER	3.0
1	S	361	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	190	GLY	3.0
1	M	220	PRO	3.0
3	O	181	LEU	3.0
4	F	212	GLU	3.0
4	Q	34	TRP	3.0
1	S	374	HIS	3.0
3	O	129	THR	3.0
4	W	20	LEU	3.0
3	K	80	PRO	3.0
3	U	127	SER	3.0
3	X	134	CYS	3.0
3	G	31	SER	3.0
4	Q	45	LEU	3.0
3	O	79	GLN	3.0
1	V	49	ASN	3.0
1	I	452	LEU	3.0
1	M	454	LEU	3.0
4	H	132	SER	3.0
4	Q	132	SER	3.0
3	G	105	GLU	3.0
3	D	87	TYR	3.0
4	J	187	SER	3.0
4	W	152	VAL	3.0
4	T	213	PRO	3.0
1	E	492	GLU	3.0
4	N	206	LYS	3.0
4	N	147	PRO	2.9
3	K	202	SER	2.9
4	F	38	ARG	2.9
3	U	86	TYR	2.9
1	E	50	THR	2.9
4	J	111	VAL	2.9
4	F	92	CYS	2.9
3	R	148	TRP	2.9
1	S	242	VAL	2.9
4	C	179	SER	2.9
4	J	106	GLY	2.9
1	V	100	MET	2.9
4	Q	54	ASN	2.9
3	O	105	GLU	2.9
3	O	205	VAL	2.9
4	H	59	TYR	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	132	SER	2.9
4	T	95	ARG	2.9
1	M	483	LEU	2.9
4	Q	48	ILE	2.9
3	R	130	ALA	2.9
3	O	193	ALA	2.9
1	A	381	GLU	2.9
4	J	186	SER	2.9
1	P	217	TYR	2.9
3	D	200	GLY	2.9
3	L	158	ASN	2.9
4	C	193	THR	2.9
1	E	350	ARG	2.9
4	T	57	PRO	2.9
1	V	286	VAL	2.9
4	N	159	LEU	2.9
1	B	472	GLY	2.9
1	E	488	VAL	2.9
1	E	381	GLU	2.9
1	S	390	LEU	2.9
3	G	143	GLU	2.9
3	X	87	TYR	2.8
3	D	78	LEU	2.8
1	B	349	LEU	2.8
3	L	196	VAL	2.8
3	O	146	VAL	2.8
4	Q	175	LEU	2.8
4	H	180	SER	2.8
4	C	34	TRP	2.8
1	E	346	VAL	2.8
1	V	342	LEU	2.8
4	J	142	VAL	2.8
4	J	48	ILE	2.8
4	F	95	ARG	2.8
4	W	173	SER	2.8
4	N	17	THR	2.8
1	V	381	GLU	2.8
3	D	182	SER	2.8
3	O	148	TRP	2.8
3	L	38	GLN	2.8
3	G	48	ILE	2.8
4	J	78	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	349	LEU	2.8
1	P	286	VAL	2.8
3	X	46	LEU	2.8
4	Q	82	LEU	2.8
1	B	285	ILE	2.8
3	R	113	PRO	2.8
1	S	349	LEU	2.8
3	L	132	VAL	2.8
1	B	492	GLU	2.8
1	M	100	MET	2.8
3	G	104	LEU	2.8
3	X	61	ARG	2.8
3	X	118	PHE	2.8
3	R	179	LEU	2.8
3	X	183	LYS	2.8
2	v	17	GLY	2.8
3	O	85	THR	2.8
4	J	21	THR	2.8
4	J	91	PHE	2.8
4	J	152	VAL	2.8
1	S	272	ILE	2.8
4	T	184	VAL	2.8
3	X	165	GLU	2.8
4	C	98	TRP	2.8
1	B	457	ASP	2.8
4	N	148	GLU	2.7
4	T	185	PRO	2.8
3	G	129	THR	2.7
4	N	194	TYR	2.7
3	O	206	THR	2.7
4	F	184	VAL	2.7
4	H	179	SER	2.7
4	H	69	ILE	2.7
4	T	69	ILE	2.7
1	B	470	PRO	2.7
3	U	110	VAL	2.7
1	V	217	TYR	2.7
3	K	195	GLU	2.7
4	N	150	VAL	2.7
3	G	180	THR	2.7
3	U	21	ILE	2.7
1	E	217	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	186	TYR	2.7
1	M	342	LEU	2.7
3	O	40	PRO	2.7
3	L	117	ILE	2.7
3	O	36	TYR	2.7
4	W	123	PRO	2.7
3	X	208	SER	2.7
4	J	124	LEU	2.7
4	Q	108	LEU	2.7
3	X	149	LYS	2.7
4	W	11	LEU	2.7
1	I	361	PHE	2.7
1	M	487	LYS	2.7
4	C	10	GLY	2.7
3	R	154	LEU	2.7
4	J	150	VAL	2.7
4	N	141	LEU	2.7
4	W	4	LEU	2.7
1	B	87	GLU	2.7
4	N	180	SER	2.7
1	E	69	TRP	2.7
4	J	138	LEU	2.7
4	J	141	LEU	2.7
3	K	192	TYR	2.7
1	S	288	LEU	2.7
3	U	117	ILE	2.7
3	X	75	ILE	2.7
1	E	288	LEU	2.7
3	D	47	VAL	2.7
4	H	4	LEU	2.7
4	H	45	LEU	2.7
3	X	122	ASP	2.7
1	B	240	LYS	2.6
3	K	151	ASP	2.6
3	X	142	ARG	2.6
4	F	33	TYR	2.6
4	Q	165	THR	2.6
1	S	93	PHE	2.6
3	X	144	ALA	2.6
3	O	117	ILE	2.6
4	W	17	THR	2.6
4	J	95	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	H	29	LEU	2.6
4	N	125	ALA	2.6
2	i	18	ARG	2.6
1	B	454	LEU	2.6
3	X	94	LEU	2.6
3	R	27	GLN	2.6
4	N	157	GLY	2.6
1	A	345	VAL	2.6
1	B	392	ASN	2.6
4	F	214	LYS	2.6
4	C	80	LEU	2.6
3	X	124	GLN	2.6
3	G	115	VAL	2.6
3	X	182	SER	2.6
4	W	120	SER	2.6
1	B	60	ALA	2.6
3	X	125	LEU	2.6
4	J	140	CYS	2.6
1	B	409	ILE	2.6
1	I	408	SER	2.6
4	T	210	LYS	2.6
2	b	27	VAL	2.6
3	D	19	VAL	2.6
4	N	149	PRO	2.6
1	E	477	ASP	2.6
1	I	324	GLY	2.6
3	R	186	TYR	2.6
1	E	107	ASP	2.6
4	N	70	SER	2.5
1	E	93	PHE	2.5
1	E	272	ILE	2.5
1	M	288	LEU	2.5
3	G	197	THR	2.5
3	K	207	LYS	2.5
4	C	110	THR	2.5
4	J	90	TYR	2.5
4	T	183	THR	2.5
3	K	201	LEU	2.5
1	I	345	VAL	2.5
3	X	198	HIS	2.5
1	S	284	ILE	2.5
4	W	214	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	T	27	GLU	2.5
3	L	168	SER	2.5
4	F	121	VAL	2.5
4	Q	184	VAL	2.5
4	W	159	LEU	2.5
3	G	54	LEU	2.5
3	R	175	LEU	2.5
4	T	119	PRO	2.5
1	B	486	TYR	2.5
3	K	118	PHE	2.5
3	D	163	VAL	2.5
4	W	162	GLY	2.5
4	W	196	CYS	2.5
3	U	141	PRO	2.5
3	D	145	LYS	2.5
3	U	123	GLU	2.5
1	B	443	ILE	2.5
4	F	98	TRP	2.5
1	E	423	ILE	2.5
3	D	151	ASP	2.5
2	m	27	VAL	2.5
4	F	103	TRP	2.5
3	K	179	LEU	2.5
4	Q	92	CYS	2.5
1	A	324	GLY	2.5
3	K	29	ILE	2.5
3	O	190	LYS	2.5
3	R	55	GLN	2.5
3	X	166	GLN	2.5
4	H	3	GLN	2.5
4	H	139	GLY	2.5
3	K	123	GLU	2.4
3	D	194	CYS	2.4
3	G	152	ASN	2.4
1	M	253	PRO	2.4
1	B	477	ASP	2.4
3	D	177	SER	2.4
4	Q	170	LEU	2.4
3	O	20	THR	2.4
3	R	126	LYS	2.4
4	Q	207	VAL	2.4
1	M	52	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	106	GLY	2.4
1	I	381	GLU	2.4
1	E	91	GLU	2.4
4	C	132	SER	2.4
4	W	50	GLU	2.4
4	F	80	LEU	2.4
3	O	186	TYR	2.4
4	C	69	ILE	2.4
3	K	1	ASP	2.4
4	H	130	SER	2.4
1	E	287	GLN	2.4
3	U	33	LEU	2.4
4	N	68	THR	2.4
4	N	124	LEU	2.4
4	F	90	TYR	2.4
4	T	194	TYR	2.4
3	U	143	GLU	2.4
4	Q	181	VAL	2.4
4	Q	97	ASN	2.4
3	D	143	GLU	2.4
3	K	55	GLN	2.4
1	E	468	PHE	2.4
3	U	35	TRP	2.4
4	J	126	PRO	2.4
4	J	173	SER	2.4
4	W	198	VAL	2.4
1	S	81	PRO	2.4
2	v	18	ARG	2.4
1	M	374	HIS	2.4
1	P	420	ILE	2.4
3	U	62	PHE	2.4
3	X	120	PRO	2.4
3	D	14	SER	2.4
3	O	168	SER	2.4
1	B	46	LYS	2.4
1	E	376	PHE	2.4
3	R	2	ILE	2.4
4	Q	46	GLU	2.4
4	C	12	LEU	2.3
3	K	48	ILE	2.3
3	O	143	GLU	2.3
4	Q	121	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	W	68	THR	2.3
1	I	288	LEU	2.3
1	V	471	GLY	2.3
3	X	40	PRO	2.3
1	I	492	GLU	2.3
4	H	95	ARG	2.3
4	H	111	VAL	2.3
1	A	271	MET	2.3
4	C	136	ALA	2.3
3	G	142	ARG	2.3
4	Q	55	GLY	2.3
4	J	67	VAL	2.3
1	B	78	ASP	2.3
3	D	107	LYS	2.3
4	F	82	LEU	2.3
1	P	361	PHE	2.3
4	J	100(C)	PHE	2.3
3	X	81	GLU	2.3
4	W	183	THR	2.3
3	L	136	LEU	2.3
3	X	86	TYR	2.3
1	A	259	LEU	2.3
3	K	35	TRP	2.3
4	N	132	SER	2.3
1	M	390	LEU	2.3
3	G	147	GLN	2.3
3	G	166	GLN	2.3
3	X	73	LEU	2.3
1	M	345	VAL	2.3
1	P	333	VAL	2.3
4	N	37	VAL	2.3
2	a	18	ARG	2.3
4	W	81	ASN	2.3
3	X	209	PHE	2.3
3	X	20	THR	2.3
4	F	126	PRO	2.3
4	H	181	VAL	2.3
4	C	198	VAL	2.3
1	P	342	LEU	2.3
1	M	381	GLU	2.3
4	C	59	TYR	2.3
3	O	19	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	Q	28	SER	2.3
4	Q	115	SER	2.3
4	W	142	VAL	2.3
3	O	94	LEU	2.3
4	C	107	THR	2.3
3	L	147	GLN	2.3
3	D	127	SER	2.3
3	X	48	ILE	2.3
4	N	27	GLU	2.3
4	T	37	VAL	2.3
1	P	259	LEU	2.2
4	F	71	LEU	2.2
4	Q	70	SER	2.2
1	M	486	TYR	2.2
4	F	198	VAL	2.2
1	P	405	GLY	2.2
2	s	18	ARG	2.2
1	P	253	PRO	2.2
3	U	198	HIS	2.2
4	C	141	LEU	2.2
3	X	153	ALA	2.2
3	O	179	LEU	2.2
1	A	49	ASN	2.2
1	I	270	VAL	2.2
3	X	123	GLU	2.2
4	F	189	LEU	2.2
3	G	126	LYS	2.2
1	B	80	SER	2.2
1	P	381	GLU	2.2
2	v	16	LEU	2.2
3	R	78	LEU	2.2
3	X	164	THR	2.2
1	E	105	HIS	2.2
1	P	419	ARG	2.2
3	X	201	LEU	2.2
4	F	152	VAL	2.2
1	I	486	TYR	2.2
3	K	208	SER	2.2
4	F	170	LEU	2.2
4	H	78	PHE	2.2
4	N	151	THR	2.2
4	T	152	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	345	VAL	2.2
3	K	137	ASN	2.2
4	N	178	LEU	2.2
4	Q	1	GLN	2.2
3	X	179	LEU	2.2
4	J	5	GLN	2.2
3	L	163	VAL	2.2
4	F	211	VAL	2.2
1	A	52	LEU	2.2
3	R	158	ASN	2.2
1	A	346	VAL	2.2
4	H	129	LYS	2.2
4	J	80	LEU	2.2
1	S	324	GLY	2.2
3	X	116	PHE	2.2
4	H	91	PHE	2.2
4	F	131	THR	2.2
4	J	155	ASN	2.2
4	J	196	CYS	2.2
1	V	273	ARG	2.2
1	A	351	LYS	2.2
3	R	177	SER	2.2
3	U	144	ALA	2.2
3	X	13	ALA	2.2
1	M	406	THR	2.2
1	E	199	SER	2.2
1	M	274	SER	2.2
4	F	113	SER	2.2
1	A	454	LEU	2.1
4	C	195	ILE	2.1
4	Q	183	THR	2.1
3	G	205	VAL	2.1
3	U	112	ALA	2.1
1	B	79	PRO	2.1
3	O	165	GLU	2.1
1	M	383	PHE	2.1
1	P	357	ASN	2.1
1	A	482	GLU	2.1
4	C	73	MET	2.1
3	K	78	LEU	2.1
4	C	209	LYS	2.1
1	I	341	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	273	ARG	2.1
2	e	22	THR	2.1
1	B	49	ASN	2.1
1	E	261	LEU	2.1
4	T	143	LYS	2.1
1	A	121	GLN	2.1
4	Q	180	SER	2.1
1	P	86	MET	2.1
4	Q	209	LYS	2.1
3	K	24	ARG	2.1
4	N	85	ALA	2.1
3	K	2	ILE	2.1
4	T	124	LEU	2.1
1	I	300	ASN	2.1
4	H	97	ASN	2.1
1	I	453	ILE	2.1
4	C	134	GLY	2.1
1	M	416	LEU	2.1
1	V	99	ASN	2.1
3	D	183	LYS	2.1
4	W	54	ASN	2.1
3	G	26	SER	2.1
4	T	35	SER	2.1
4	T	200	HIS	2.1
3	U	25	ALA	2.1
4	T	48	ILE	2.1
1	A	93	PHE	2.1
4	J	209	LYS	2.1
1	E	260	LEU	2.1
3	U	201	LEU	2.1
1	E	210	PHE	2.1
1	P	407	ALA	2.1
3	O	197	THR	2.1
3	D	146	VAL	2.1
4	T	121	VAL	2.1
3	L	14	SER	2.1
4	C	214	LYS	2.1
1	A	226	LEU	2.1
1	I	217	TYR	2.1
4	N	29	LEU	2.1
1	B	361	PHE	2.1
4	W	143	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	250	GLY	2.1
3	L	131	SER	2.1
4	C	8	GLY	2.1
4	W	180	SER	2.1
1	E	239	CYS	2.1
4	Q	100(C)	PHE	2.1
3	U	186	TYR	2.1
4	N	48	ILE	2.1
3	G	199	GLN	2.1
4	T	98	TRP	2.0
3	X	146	VAL	2.0
4	J	184	VAL	2.0
3	K	94	LEU	2.0
4	Q	109	VAL	2.0
4	T	136	ALA	2.0
4	W	35	SER	2.0
3	G	194	CYS	2.0
3	K	91	LEU	2.0
1	B	406	THR	2.0
4	H	131	THR	2.0
4	J	127	SER	2.0
4	W	70	SER	2.0
4	C	189	LEU	2.0
1	B	282	LYS	2.0
1	M	492	GLU	2.0
4	T	111	VAL	2.0
1	E	451	GLY	2.0
3	D	52	SER	2.0
4	N	115	SER	2.0
3	L	205	VAL	2.0
4	N	121	VAL	2.0
3	D	142	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	U2X	p	23	19/20	0.80	0.37	-	106,113,127,130	0
2	DPR	b	21	7/8	0.94	0.18	-	165,166,170,173	0
2	DPR	v	21	7/8	0.95	0.39	-	170,171,176,180	0
2	U2X	a	23	19/20	0.85	0.44	-	130,136,145,145	0
2	U2X	v	23	19/20	0.93	0.33	-	146,156,181,182	0
2	U2X	i	23	19/20	0.86	0.43	-	133,139,150,152	0
4	OAS	F	30	6/10	0.83	0.13	-	248,273,281,281	0
4	OAS	C	30	9/10	0.92	0.28	-	155,165,179,180	0
2	DPR	i	21	7/8	0.94	0.26	-	136,137,141,144	0
2	U2X	b	23	19/20	0.81	0.39	-	131,154,176,177	0
4	OAS	Q	30	6/10	0.68	0.30	-	246,262,273,274	0
4	OAS	J	30	6/10	0.82	0.12	-	164,236,245,246	0
2	DPR	a	21	7/8	0.95	0.17	-	146,147,150,151	0
2	DPR	p	21	7/8	0.93	0.25	-	123,126,133,136	0
2	U2X	m	23	19/20	0.91	0.35	-	155,164,181,184	0
4	OAS	W	30	9/10	0.71	0.38	-	201,211,216,219	0
2	DPR	s	21	7/8	0.95	0.17	-	151,152,155,158	0
4	OAS	H	30	9/10	0.89	0.14	-	172,176,180,182	0
4	OAS	N	30	6/10	0.82	0.18	-	179,233,246,251	0
2	DPR	m	21	7/8	0.97	0.26	-	173,175,182,187	0
2	DPR	e	21	7/8	0.98	0.33	-	176,177,180,182	0
2	U2X	e	23	19/20	0.78	0.42	-	175,179,184,185	0
4	OAS	T	30	9/10	0.86	0.23	-	156,170,195,200	0
2	U2X	s	23	19/20	0.84	0.37	-	146,152,160,160	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	A	503	14/15	0.89	0.35	1.33	152,167,177,182	0
5	NAG	S	501	14/15	0.84	0.36	0.71	154,162,168,171	0
5	NAG	A	501	14/15	0.87	0.36	0.58	127,136,143,144	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	E	502	14/15	0.74	0.28	0.40	190,201,211,212	0
5	NAG	V	501	14/15	0.93	0.38	0.40	153,158,163,165	0
5	NAG	P	502	14/15	0.75	0.26	0.35	208,216,230,231	0
5	NAG	E	501	14/15	0.84	0.38	0.27	204,207,209,209	0
5	NAG	I	502	14/15	0.58	0.43	0.22	183,189,198,199	0
5	NAG	S	503	14/15	0.89	0.29	0.15	202,210,214,216	0
5	NAG	M	501	14/15	0.86	0.42	0.14	178,180,182,185	0
5	NAG	I	504	14/15	0.80	0.26	0.14	176,180,185,186	0
5	NAG	B	501	14/15	0.80	0.28	-0.09	152,161,168,170	0
5	NAG	S	502	14/15	0.86	0.18	-0.30	230,238,252,259	0
5	NAG	I	501	14/15	0.93	0.23	-0.43	161,165,172,173	0
5	NAG	P	501	14/15	0.91	0.23	-0.48	153,165,177,177	0
5	NAG	A	502	14/15	0.88	0.20	-0.69	184,189,200,200	0
5	NAG	B	502	14/15	0.86	0.12	-0.82	219,232,245,249	0
5	NAG	A	504	14/15	0.84	0.14	-	184,188,192,195	0
5	NAG	I	503	14/15	0.86	0.21	-	194,202,208,209	0

6.5 Other polymers

There are no such residues in this entry.