



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2023 – 08:15 PM EDT

PDB ID : 7S7I  
Title : Crystal structure of Fab in complex with MICA alpha3 domain  
Authors : Lee, P.S.; Strop, P.  
Deposited on : 2021-09-16  
Resolution : 2.40 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

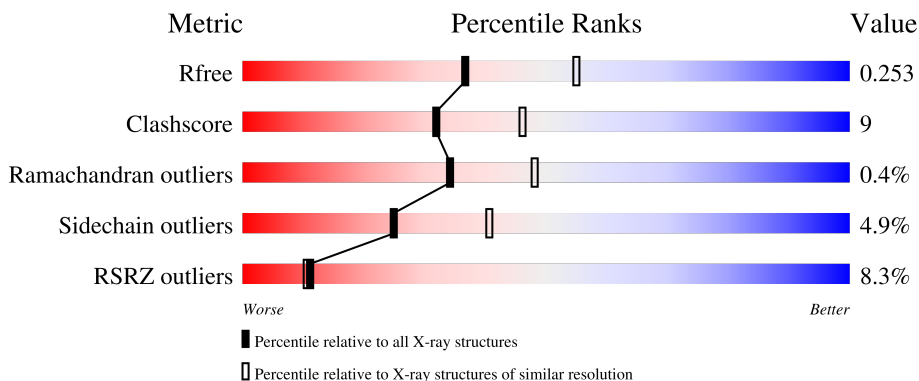
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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.



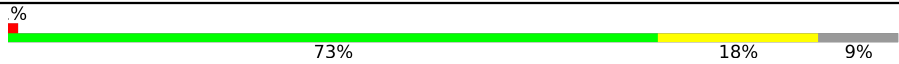




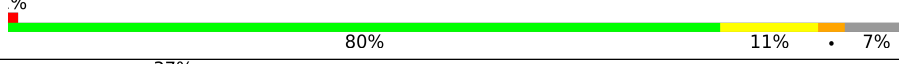
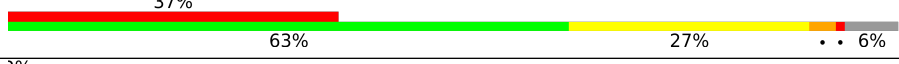
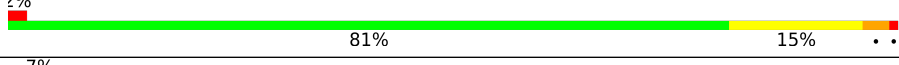
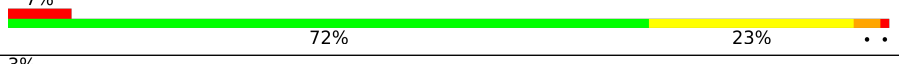



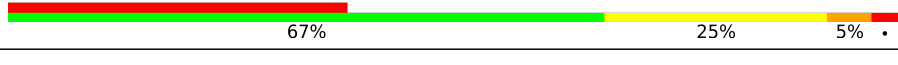
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	103	 72% 17% • 9%
1	B	103	 77% 15% • 8%
1	C	103	 4% 75% 12% • • 10%
1	D	103	 14% 64% 22% • • 10%
1	E	103	 % 69% 19% • 9%

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Mol	Chain	Length	Quality of chain
1	F	103	
2	H	230	
2	I	230	
2	J	230	
2	U	230	
2	W	230	
2	Y	230	
3	L	214	
3	M	214	
3	N	214	
3	V	214	
3	X	214	
3	Z	214	

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	EDO	B	402	-	-	X	-
5	EDO	E	402	-	-	X	-
5	EDO	U	301	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 24458 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MHC class I chain-related protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	94	741	455	136	145	5	0	0	0
1	B	95	747	458	137	147	5	0	0	0
1	C	93	735	452	135	143	5	0	0	0
1	D	93	735	452	135	143	5	0	0	0
1	E	94	741	455	136	145	5	0	0	0
1	F	94	741	455	136	145	5	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLY	-	expression tag	UNP H9CTV0
A	203	SER	-	expression tag	UNP H9CTV0
A	299	HIS	-	expression tag	UNP H9CTV0
A	300	HIS	-	expression tag	UNP H9CTV0
A	301	HIS	-	expression tag	UNP H9CTV0
A	302	HIS	-	expression tag	UNP H9CTV0
A	303	HIS	-	expression tag	UNP H9CTV0
A	304	HIS	-	expression tag	UNP H9CTV0
B	202	GLY	-	expression tag	UNP H9CTV0
B	203	SER	-	expression tag	UNP H9CTV0
B	299	HIS	-	expression tag	UNP H9CTV0
B	300	HIS	-	expression tag	UNP H9CTV0
B	301	HIS	-	expression tag	UNP H9CTV0
B	302	HIS	-	expression tag	UNP H9CTV0
B	303	HIS	-	expression tag	UNP H9CTV0
B	304	HIS	-	expression tag	UNP H9CTV0
C	202	GLY	-	expression tag	UNP H9CTV0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	203	SER	-	expression tag	UNP H9CTV0
C	299	HIS	-	expression tag	UNP H9CTV0
C	300	HIS	-	expression tag	UNP H9CTV0
C	301	HIS	-	expression tag	UNP H9CTV0
C	302	HIS	-	expression tag	UNP H9CTV0
C	303	HIS	-	expression tag	UNP H9CTV0
C	304	HIS	-	expression tag	UNP H9CTV0
D	202	GLY	-	expression tag	UNP H9CTV0
D	203	SER	-	expression tag	UNP H9CTV0
D	299	HIS	-	expression tag	UNP H9CTV0
D	300	HIS	-	expression tag	UNP H9CTV0
D	301	HIS	-	expression tag	UNP H9CTV0
D	302	HIS	-	expression tag	UNP H9CTV0
D	303	HIS	-	expression tag	UNP H9CTV0
D	304	HIS	-	expression tag	UNP H9CTV0
E	202	GLY	-	expression tag	UNP H9CTV0
E	203	SER	-	expression tag	UNP H9CTV0
E	299	HIS	-	expression tag	UNP H9CTV0
E	300	HIS	-	expression tag	UNP H9CTV0
E	301	HIS	-	expression tag	UNP H9CTV0
E	302	HIS	-	expression tag	UNP H9CTV0
E	303	HIS	-	expression tag	UNP H9CTV0
E	304	HIS	-	expression tag	UNP H9CTV0
F	202	GLY	-	expression tag	UNP H9CTV0
F	203	SER	-	expression tag	UNP H9CTV0
F	299	HIS	-	expression tag	UNP H9CTV0
F	300	HIS	-	expression tag	UNP H9CTV0
F	301	HIS	-	expression tag	UNP H9CTV0
F	302	HIS	-	expression tag	UNP H9CTV0
F	303	HIS	-	expression tag	UNP H9CTV0
F	304	HIS	-	expression tag	UNP H9CTV0

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	H	213	Total	C	N	O	S	0	0	0
			1618	1023	274	315	6			
2	I	211	Total	C	N	O	S	0	0	0
			1606	1017	272	311	6			
2	J	214	Total	C	N	O	S	0	0	0
			1622	1025	275	316	6			
2	U	212	Total	C	N	O	S	0	0	0
			1610	1019	273	312	6			

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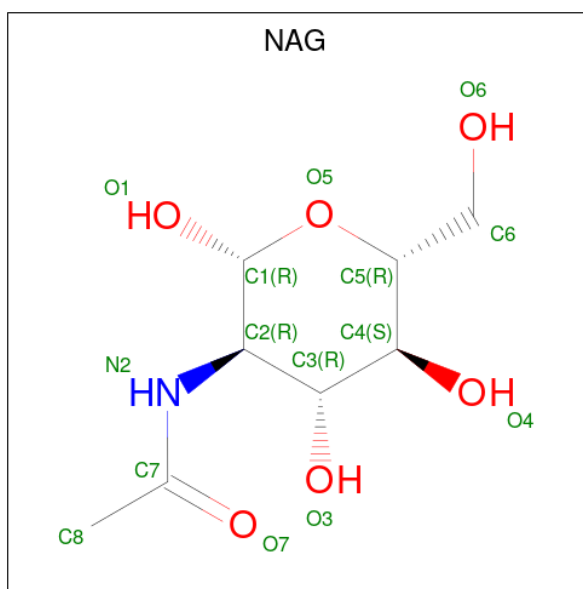
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	215	Total	C	N	O	S	0	0	0
			1633	1032	277	318	6			
2	Y	217	Total	C	N	O	S	0	0	0
			1641	1036	279	320	6			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			
3	M	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			
3	N	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			
3	V	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			
3	X	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			
3	Z	213	Total	C	N	O	S	0	0	0
			1630	1020	275	331	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



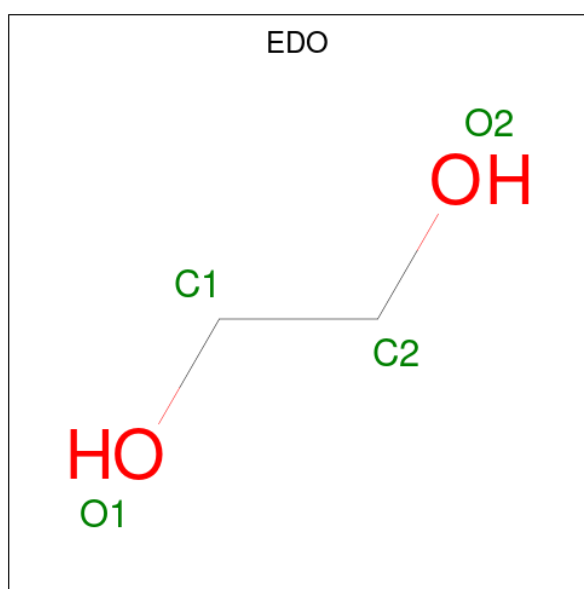
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	L	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	U	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	58	Total 58	O 58	0	0
6	L	22	Total 22	O 22	0	0
6	B	28	Total 28	O 28	0	0
6	I	54	Total 54	O 54	0	0
6	M	13	Total 13	O 13	0	0
6	C	9	Total 9	O 9	0	0
6	J	52	Total 52	O 52	0	0
6	N	16	Total 16	O 16	0	0
6	D	6	Total 6	O 6	0	0
6	U	31	Total 31	O 31	0	0
6	V	11	Total 11	O 11	0	0
6	E	22	Total 22	O 22	0	0
6	W	30	Total 30	O 30	0	0
6	X	12	Total 12	O 12	0	0
6	F	14	Total 14	O 14	0	0
6	Y	16	Total 16	O 16	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: MHC class I chain-related protein A

Chain A: 




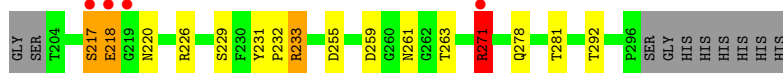
- Molecule 1: MHC class I chain-related protein A

Chain B: 



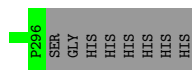
- Molecule 1: MHC class I chain-related protein A

Chain C: 



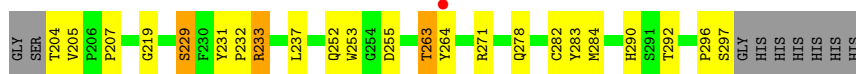
- Molecule 1: MHC class I chain-related protein A

Chain D: 

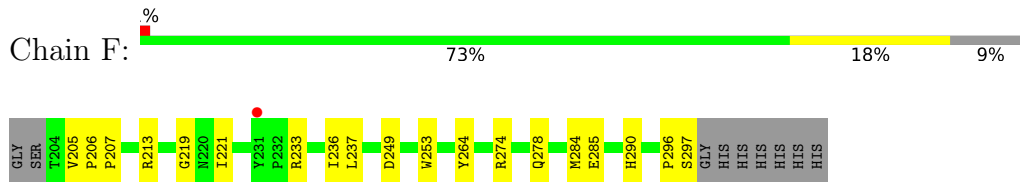


- Molecule 1: MHC class I chain-related protein A

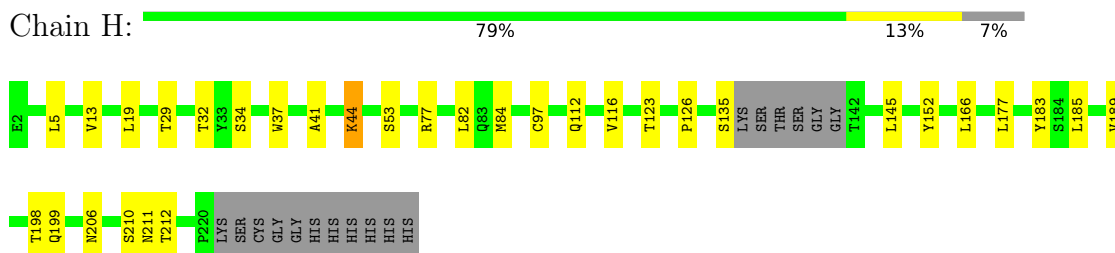
Chain E: 



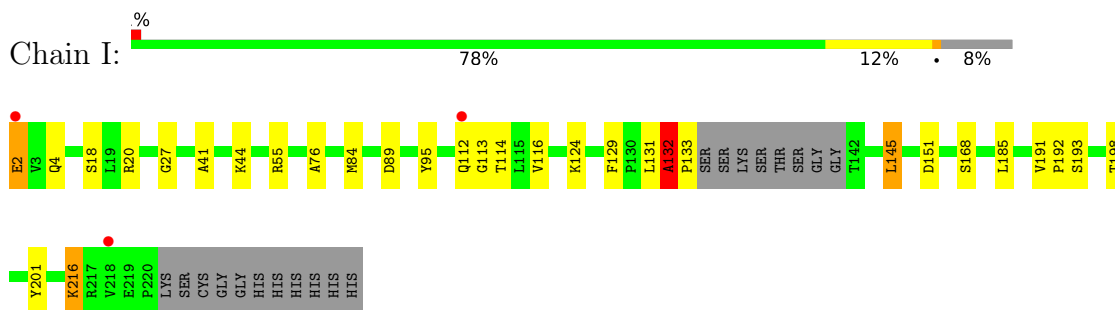
- Molecule 1: MHC class I chain-related protein A



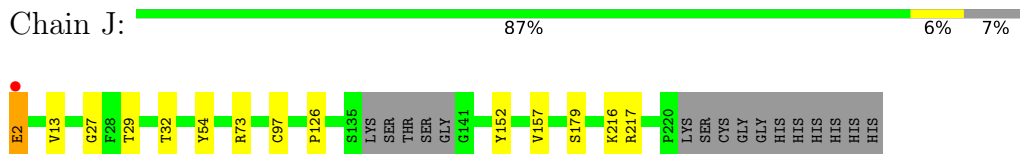
- Molecule 2: Fab heavy chain



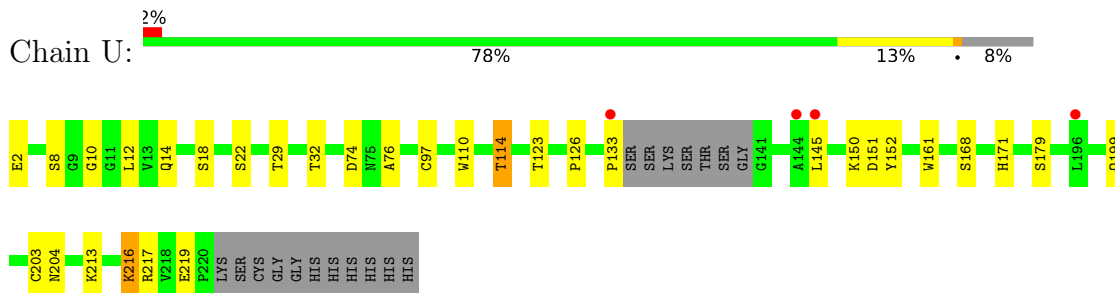
- Molecule 2: Fab heavy chain



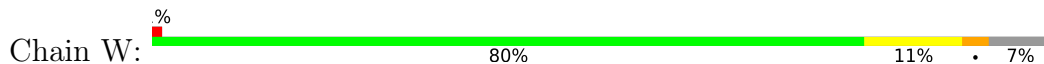
- Molecule 2: Fab heavy chain

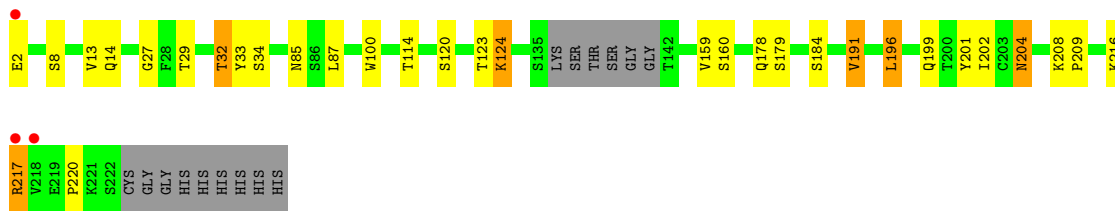


- Molecule 2: Fab heavy chain

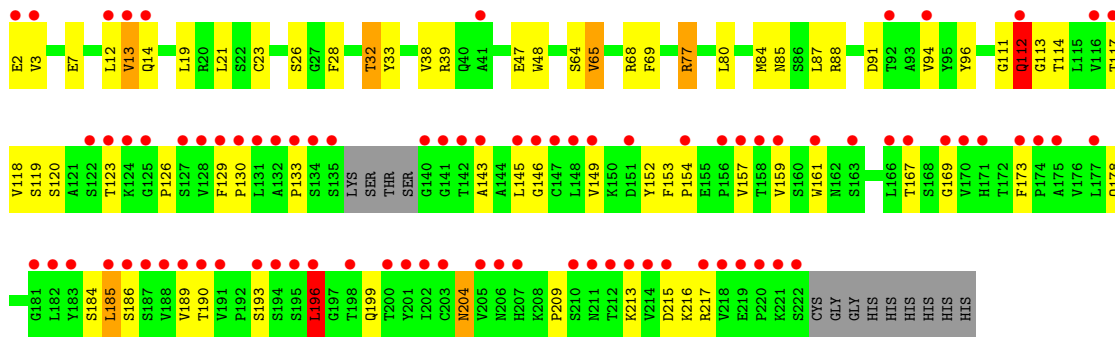


- Molecule 2: Fab heavy chain

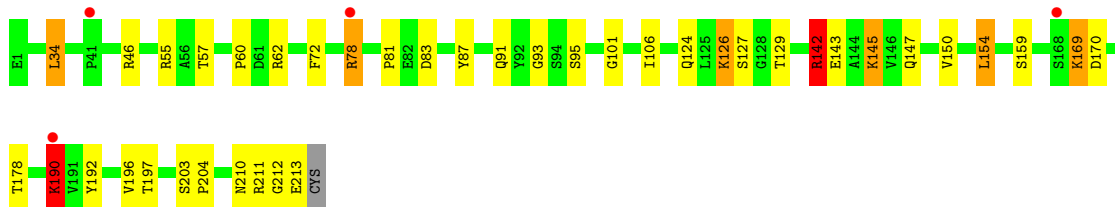
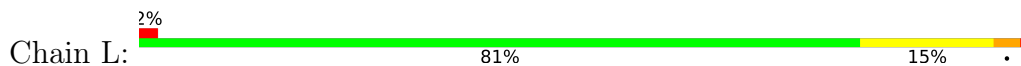




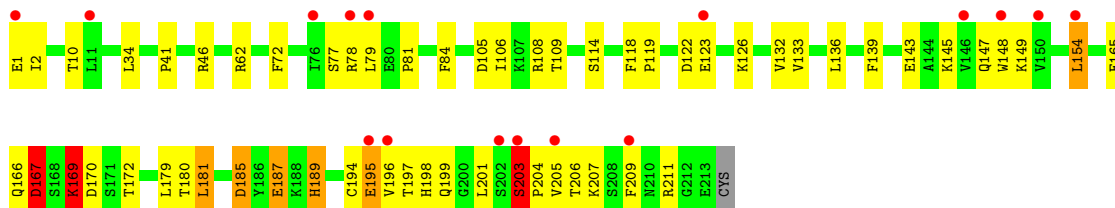
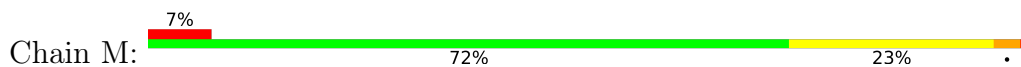
● Molecule 2: Fab heavy chain



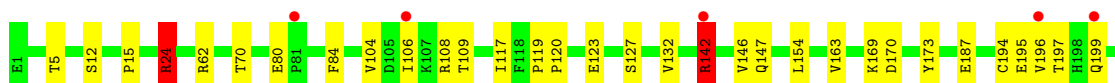
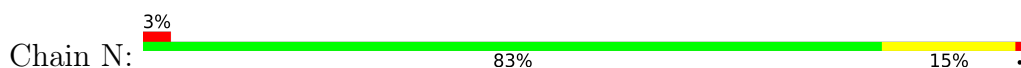
● Molecule 3: Fab light chain



● Molecule 3: Fab light chain

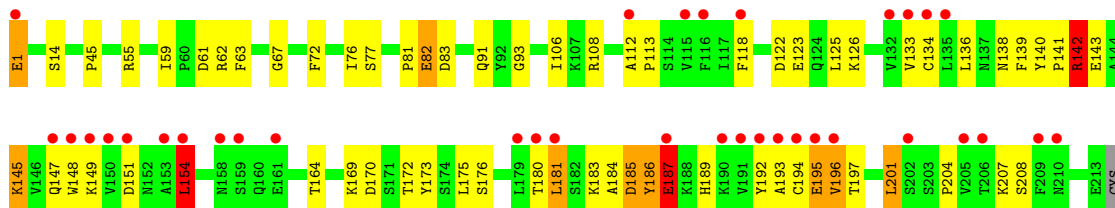


● Molecule 3: Fab light chain

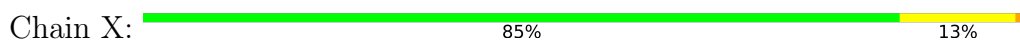




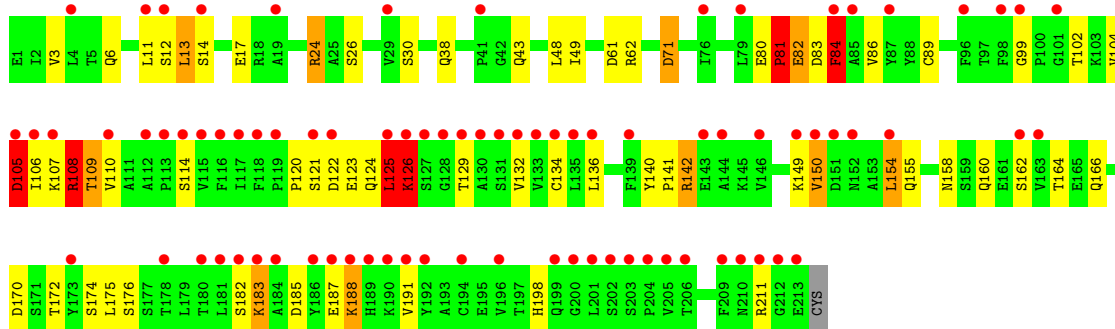
• Molecule 3: Fab light chain



• Molecule 3: Fab light chain



• Molecule 3: Fab light chain



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.78Å 170.43Å 148.89Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	44.63 – 2.40 143.26 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.63-2.40) 99.4 (143.26-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 2.40Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.220 , 0.260 0.214 , 0.253	Depositor DCC
$R_{free}$ test set	8731 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.8	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24458	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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, EDO

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	0.56	0/761	0.73	0/1040
1	B	0.55	0/767	0.73	0/1048
1	C	0.53	0/755	0.87	3/1032 (0.3%)
1	D	0.46	0/755	0.84	1/1032 (0.1%)
1	E	0.48	0/761	0.70	0/1040
1	F	0.47	0/761	0.66	0/1040
2	H	0.57	1/1659 (0.1%)	0.72	3/2260 (0.1%)
2	I	0.58	0/1647	0.87	5/2244 (0.2%)
2	J	0.56	1/1663 (0.1%)	0.69	2/2265 (0.1%)
2	U	0.49	1/1651 (0.1%)	0.70	0/2249
2	W	0.47	0/1674	0.78	3/2279 (0.1%)
2	Y	0.57	0/1682	1.01	10/2289 (0.4%)
3	L	0.51	0/1666	0.96	11/2262 (0.5%)
3	M	0.53	0/1666	1.05	11/2262 (0.5%)
3	N	0.51	1/1666 (0.1%)	0.88	10/2262 (0.4%)
3	V	0.61	3/1666 (0.2%)	1.04	15/2262 (0.7%)
3	X	0.52	0/1666	0.91	8/2262 (0.4%)
3	Z	0.53	2/1666 (0.1%)	1.26	19/2262 (0.8%)
All	All	0.53	9/24532 (0.0%)	0.89	101/33390 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	D	0	2
2	I	0	2
2	Y	0	2
3	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	M	0	3
3	N	0	1
3	V	0	3
3	X	0	3
3	Z	0	4
All	All	0	24

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	154	LEU	CG-CD1	7.52	1.79	1.51
2	J	97	CYS	CB-SG	-6.28	1.71	1.82
3	V	142	ARG	CB-CG	-6.15	1.35	1.52
2	H	97	CYS	CB-SG	-5.92	1.72	1.81
3	N	199	GLN	CG-CD	5.43	1.63	1.51
3	V	82	GLU	CG-CD	-5.27	1.44	1.51
3	Z	150	VAL	CB-CG2	5.21	1.63	1.52
3	Z	154	LEU	CG-CD1	-5.13	1.32	1.51
2	U	97	CYS	CB-SG	-5.12	1.73	1.81

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	154	LEU	CB-CG-CD1	-28.41	62.71	111.00
3	Z	154	LEU	CB-CG-CD2	18.15	141.85	111.00
3	M	154	LEU	CB-CG-CD2	-17.89	80.59	111.00
2	Y	196	LEU	CB-CG-CD2	-17.42	81.39	111.00
3	V	154	LEU	CB-CG-CD2	15.10	136.67	111.00
3	L	78	ARG	CB-CG-CD	-14.09	74.96	111.60
3	Z	126	LYS	CA-CB-CG	-12.87	85.09	113.40
2	Y	196	LEU	CB-CG-CD1	12.68	132.56	111.00
3	L	126	LYS	CB-CA-C	-12.30	85.80	110.40
3	N	24	ARG	CB-CG-CD	-12.23	79.80	111.60
3	L	78	ARG	CA-CB-CG	12.15	140.13	113.40
3	N	24	ARG	CG-CD-NE	11.91	136.82	111.80
3	M	167	ASP	CB-CG-OD2	-11.88	107.61	118.30
3	Z	24	ARG	CG-CD-NE	11.72	136.41	111.80
3	N	142	ARG	CA-CB-CG	11.57	138.86	113.40
2	Y	112	GLN	CA-CB-CG	11.54	138.79	113.40
3	L	126	LYS	CA-CB-CG	11.29	138.23	113.40
3	V	142	ARG	CG-CD-NE	-11.22	88.24	111.80
2	I	132	ALA	C-N-CD	-11.20	95.96	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	46	ARG	CB-CG-CD	-10.73	83.69	111.60
2	W	196	LEU	CB-CG-CD2	-10.56	93.05	111.00
3	X	46	ARG	CG-CD-NE	10.49	133.82	111.80
3	Z	84	PHE	CB-CG-CD1	-9.83	113.92	120.80
3	X	123	GLU	CA-CB-CG	9.48	134.26	113.40
3	V	123	GLU	CB-CA-C	-9.39	91.61	110.40
2	Y	112	GLN	C-N-CA	9.05	141.30	122.30
3	L	78	ARG	CD-NE-CZ	-8.65	111.49	123.60
3	X	78	ARG	NE-CZ-NH1	8.64	124.62	120.30
3	M	154	LEU	CB-CG-CD1	8.21	124.95	111.00
3	Z	105	ASP	CB-CA-C	-8.02	94.36	110.40
3	X	123	GLU	N-CA-CB	7.99	124.99	110.60
3	Z	154	LEU	CA-CB-CG	7.79	133.21	115.30
3	X	24	ARG	CB-CG-CD	7.75	131.74	111.60
3	M	167	ASP	CB-CG-OD1	7.61	125.14	118.30
3	N	195	GLU	CA-CB-CG	7.51	129.92	113.40
2	I	131	LEU	C-N-CA	7.38	140.15	121.70
3	Z	154	LEU	CD1-CG-CD2	-7.31	88.56	110.50
3	V	1	GLU	CG-CD-OE2	-7.23	103.83	118.30
3	V	187	GLU	CA-CB-CG	7.04	128.88	113.40
1	D	226	ARG	CB-CA-C	-6.99	96.43	110.40
3	V	142	ARG	CB-CG-CD	6.91	129.56	111.60
3	L	126	LYS	CD-CE-NZ	-6.84	95.96	111.70
3	Z	24	ARG	CD-NE-CZ	-6.84	114.02	123.60
3	M	169	LYS	CA-CB-CG	6.82	128.40	113.40
3	M	123	GLU	N-CA-CB	6.81	122.86	110.60
3	V	142	ARG	CA-CB-CG	-6.81	98.43	113.40
3	Z	84	PHE	CB-CG-CD2	6.79	125.56	120.80
3	Z	108	ARG	CG-CD-NE	-6.78	97.56	111.80
3	L	145	LYS	CD-CE-NZ	-6.67	96.35	111.70
2	I	112	GLN	CA-CB-CG	-6.67	98.73	113.40
3	M	154	LEU	CA-CB-CG	6.44	130.12	115.30
3	Z	125	LEU	C-N-CA	-6.41	105.68	121.70
3	X	78	ARG	CG-CD-NE	6.26	124.94	111.80
3	N	24	ARG	NE-CZ-NH2	-6.25	117.17	120.30
3	V	82	GLU	CA-CB-CG	-6.23	99.68	113.40
2	Y	13	VAL	CG1-CB-CG2	6.22	120.86	110.90
3	Z	24	ARG	NE-CZ-NH1	6.21	123.41	120.30
3	L	78	ARG	CG-CD-NE	6.20	124.83	111.80
3	M	123	GLU	CB-CA-C	-6.20	98.00	110.40
3	L	126	LYS	N-CA-CB	6.19	121.75	110.60
3	M	207	LYS	CD-CE-NZ	6.17	125.88	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	196	LEU	CA-CB-CG	6.07	129.25	115.30
2	I	2	GLU	CA-CB-CG	6.02	126.65	113.40
3	V	145	LYS	CD-CE-NZ	-5.95	98.02	111.70
2	Y	77	ARG	CB-CG-CD	5.94	127.05	111.60
2	W	196	LEU	CB-CG-CD1	5.94	121.10	111.00
3	V	195	GLU	CA-CB-CG	5.92	126.43	113.40
3	Z	105	ASP	N-CA-CB	5.90	121.22	110.60
1	C	218	GLU	CA-CB-CG	5.90	126.37	113.40
3	L	78	ARG	CB-CA-C	-5.89	98.61	110.40
3	N	142	ARG	CD-NE-CZ	5.87	131.82	123.60
3	N	142	ARG	NE-CZ-NH2	-5.83	117.39	120.30
3	N	142	ARG	CG-CD-NE	-5.80	99.62	111.80
2	H	44	LYS	CA-CB-CG	5.78	126.11	113.40
2	J	2	GLU	CA-CB-CG	5.73	126.01	113.40
2	Y	2	GLU	CB-CA-C	-5.71	98.99	110.40
3	L	190	LYS	CB-CG-CD	-5.70	96.78	111.60
3	Z	188	LYS	CD-CE-NZ	-5.55	98.93	111.70
2	H	212	THR	OG1-CB-CG2	5.54	122.75	110.00
2	J	2	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	C	271	ARG	N-CA-CB	5.45	120.42	110.60
3	V	123	GLU	CA-CB-CG	5.45	125.39	113.40
2	Y	2	GLU	N-CA-C	5.45	125.71	111.00
1	C	271	ARG	CB-CG-CD	5.43	125.73	111.60
3	V	1	GLU	N-CA-C	5.42	125.63	111.00
2	Y	2	GLU	CA-CB-CG	-5.36	101.60	113.40
3	X	61	ASP	CB-CG-OD1	-5.34	113.49	118.30
3	M	181	LEU	CB-CG-CD2	-5.33	101.94	111.00
3	Z	108	ARG	CB-CG-CD	-5.32	97.77	111.60
3	Z	24	ARG	NE-CZ-NH2	-5.31	117.64	120.30
3	N	24	ARG	CA-CB-CG	5.30	125.06	113.40
3	V	123	GLU	N-CA-CB	5.28	120.10	110.60
3	Z	82	GLU	CA-CB-CG	5.23	124.91	113.40
2	H	185	LEU	CA-CB-CG	5.21	127.28	115.30
3	N	142	ARG	N-CA-CB	-5.20	101.25	110.60
3	Z	183	LYS	CD-CE-NZ	-5.11	99.95	111.70
2	Y	185	LEU	CA-CB-CG	5.10	127.03	115.30
3	V	1	GLU	CA-CB-CG	5.08	124.57	113.40
3	V	181	LEU	CA-CB-CG	5.06	126.93	115.30
3	M	122	ASP	CB-CG-OD2	5.04	122.83	118.30
2	I	132	ALA	N-CA-C	5.02	124.57	111.00

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	217	SER	Peptide
1	C	233	ARG	Sidechain
1	C	271	ARG	Sidechain
1	D	216	ALA	Peptide
1	D	226	ARG	Sidechain
2	I	132	ALA	Peptide
2	I	2	GLU	Peptide
3	L	142	ARG	Sidechain
3	M	167	ASP	Sidechain
3	M	187	GLU	Peptide
3	M	203	SER	Peptide
3	N	24	ARG	Sidechain
3	V	108	ARG	Sidechain
3	V	186	TYR	Peptide
3	V	194	CYS	Peptide
3	X	1	GLU	Peptide
3	X	24	ARG	Sidechain
3	X	60	PRO	Peptide
2	Y	111	GLY	Peptide
2	Y	112	GLN	Peptide
3	Z	108	ARG	Sidechain
3	Z	125	LEU	Peptide
3	Z	24	ARG	Sidechain
3	Z	81	PRO	Peptide

## 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	741	0	688	12	0
1	B	747	0	693	13	0
1	C	735	0	684	12	0
1	D	735	0	684	19	0
1	E	741	0	688	18	0
1	F	741	0	687	14	0
2	H	1618	0	1562	16	0
2	I	1606	0	1552	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	1622	0	1565	7	0
2	U	1610	0	1555	23	0
2	W	1633	0	1580	24	0
2	Y	1641	0	1585	56	0
3	L	1630	0	1581	30	0
3	M	1630	0	1581	35	0
3	N	1630	0	1581	24	0
3	V	1630	0	1581	49	0
3	X	1630	0	1581	16	0
3	Z	1630	0	1581	60	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	E	14	0	13	0	0
4	F	28	0	26	0	0
5	B	4	0	6	7	0
5	E	4	0	6	5	0
5	L	4	0	6	1	0
5	U	4	0	6	3	0
6	A	28	0	0	0	0
6	B	28	0	0	1	0
6	C	9	0	0	1	0
6	D	6	0	0	0	0
6	E	22	0	0	1	0
6	F	14	0	0	1	0
6	H	58	0	0	0	0
6	I	54	0	0	0	0
6	J	52	0	0	2	0
6	L	22	0	0	1	0
6	M	13	0	0	1	0
6	N	16	0	0	1	0
6	U	31	0	0	0	0
6	V	11	0	0	0	0
6	W	30	0	0	1	0
6	X	12	0	0	1	0
6	Y	16	0	0	1	0
All	All	24458	0	23098	419	0

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 9.

All (419) 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)
3:V:154:LEU:CG	3:V:154:LEU:CD1	1.79	1.59
3:V:142:ARG:HH22	3:V:175:LEU:HD12	1.13	1.09
5:U:301:EDO:H21	2:Y:32:THR:HG21	1.37	1.04
2:J:27:GLY:H	1:E:278:GLN:HE22	1.09	0.99
3:Z:108:ARG:HH12	3:Z:172:THR:HG23	1.28	0.97
3:M:167:ASP:OD2	3:M:169:LYS:HB2	1.66	0.94
3:M:145:LYS:HE3	3:M:147:GLN:HG3	1.49	0.94
1:A:278:GLN:HE22	2:I:27:GLY:H	1.16	0.89
1:D:222:THR:OG1	1:D:271:ARG:NH2	2.07	0.87
3:V:184:ALA:O	3:V:187:GLU:HB2	1.74	0.87
1:C:220:ASN:ND2	1:C:271:ARG:HH21	1.75	0.85
3:V:142:ARG:NH2	3:V:175:LEU:HD12	1.92	0.83
1:B:208:MET:CE	1:B:210:ASN:HD22	1.94	0.80
3:M:195:GLU:OE1	3:M:206:THR:OG1	1.97	0.80
3:M:203:SER:HB2	3:M:204:PRO:HD3	1.63	0.78
3:Z:81:PRO:O	3:Z:83:ASP:N	2.17	0.78
2:Y:96:TYR:HE1	2:Y:112:GLN:O	1.67	0.78
1:B:208:MET:HE1	1:B:210:ASN:HD22	1.48	0.77
3:N:142:ARG:NH1	3:N:163:VAL:HG11	2.00	0.77
1:C:278:GLN:OE1	2:W:27:GLY:N	2.15	0.76
1:C:217:SER:O	1:C:218:GLU:HB2	1.86	0.76
3:Z:126:LYS:HA	3:Z:183:LYS:HZ2	1.50	0.76
3:Z:108:ARG:HH12	3:Z:172:THR:CG2	1.99	0.75
3:V:147:GLN:O	3:V:195:GLU:HB3	1.87	0.75
2:Y:126:PRO:HB3	2:Y:152:TYR:HB3	1.68	0.75
5:B:402:EDO:H21	2:U:76:ALA:HB2	1.70	0.74
3:M:108:ARG:NH1	3:M:109:THR:O	2.21	0.74
3:Z:150:VAL:HG11	3:Z:155:GLN:HE22	1.52	0.73
3:Z:150:VAL:CG1	3:Z:155:GLN:HE22	2.01	0.73
3:Z:108:ARG:NH1	3:Z:172:THR:HG23	2.03	0.73
3:Z:149:LYS:HG2	3:Z:154:LEU:HD11	1.69	0.72
2:I:41:ALA:HB3	2:I:44:LYS:HG2	1.72	0.72
3:X:108:ARG:HG3	3:X:108:ARG:HH11	1.55	0.71
3:V:154:LEU:CD1	3:V:154:LEU:CB	2.69	0.71
3:L:62:ARG:NH1	3:L:83:ASP:OD2	2.21	0.70
1:E:219:GLY:HA2	5:E:402:EDO:H11	1.73	0.70
3:N:123:GLU:OE2	6:N:301:HOH:O	2.09	0.70
3:V:142:ARG:HG3	3:V:142:ARG:O	1.80	0.70
2:Y:3:VAL:HG22	2:Y:28:PHE:CD1	2.26	0.70
2:Y:112:GLN:HB3	2:Y:113:GLY:O	1.91	0.70
3:V:81:PRO:HA	3:V:106:ILE:HG13	1.73	0.70
3:M:187:GLU:OE1	3:M:211:ARG:NH2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:12:LEU:HD23	2:U:123:THR:HG22	1.74	0.69
3:V:142:ARG:HH22	3:V:175:LEU:CD1	1.97	0.69
2:Y:13:VAL:HG13	2:Y:118:VAL:HG12	1.74	0.68
2:I:76:ALA:HB2	5:E:402:EDO:H21	1.76	0.67
3:N:142:ARG:HB2	3:N:173:TYR:CD2	2.29	0.67
1:B:278:GLN:OE1	6:B:501:HOH:O	2.11	0.67
2:Y:12:LEU:HD21	2:Y:153:PHE:CE2	2.29	0.67
2:W:160:SER:OG	2:W:204:ASN:OD1	2.12	0.66
3:Z:84:PHE:HB3	3:Z:104:VAL:O	1.96	0.66
1:C:220:ASN:HD22	1:C:271:ARG:HH21	1.41	0.66
3:V:118:PHE:HB2	3:V:133:VAL:HG22	1.79	0.65
1:B:219:GLY:HA2	5:B:402:EDO:H11	1.78	0.65
3:M:1:GLU:HG3	3:M:2:ILE:N	2.12	0.65
3:Z:126:LYS:HG3	3:Z:183:LYS:NZ	2.11	0.65
1:B:285:GLU:HG2	1:B:290:HIS:CD2	2.32	0.65
1:D:259:ASP:HB2	1:D:263:THR:O	1.97	0.65
1:A:259:ASP:OD2	1:A:263:THR:OG1	2.08	0.64
2:W:2:GLU:HG2	6:W:312:HOH:O	1.95	0.64
3:M:136:LEU:HD11	3:M:196:VAL:HG11	1.79	0.64
1:F:237:LEU:HD13	1:F:284:MET:HG3	1.80	0.64
3:Z:149:LYS:HG2	3:Z:154:LEU:CD1	2.27	0.64
1:E:233:ARG:HG3	1:E:264:TYR:CE2	2.33	0.64
2:U:171:HIS:HE1	3:V:138:ASN:HD21	1.45	0.64
2:U:133:PRO:HD3	2:U:145:LEU:HB3	1.80	0.64
3:V:184:ALA:HA	3:V:187:GLU:HG3	1.78	0.64
3:Z:121:SER:O	3:Z:125:LEU:HG	1.98	0.64
3:L:190:LYS:HE3	3:L:211:ARG:HB3	1.80	0.63
3:N:142:ARG:HH12	3:N:163:VAL:HG11	1.63	0.63
2:I:191:VAL:HG21	2:I:201:TYR:OH	1.98	0.63
3:L:190:LYS:HE3	3:L:211:ARG:CA	2.28	0.63
3:Z:6:GLN:NE2	3:Z:99:GLY:HA3	2.12	0.63
3:L:190:LYS:HE3	3:L:211:ARG:N	2.14	0.63
6:J:349:HOH:O	2:W:32:THR:HG21	1.99	0.63
3:Z:6:GLN:NE2	3:Z:89:CYS:SG	2.72	0.63
2:J:2:GLU:N	6:J:301:HOH:O	2.31	0.62
3:V:154:LEU:CD1	3:V:154:LEU:CD2	2.76	0.62
2:H:29:THR:O	2:H:32:THR:HG22	1.99	0.62
3:Z:3:VAL:HG23	3:Z:26:SER:HB3	1.82	0.62
3:M:189:HIS:O	3:M:211:ARG:HD3	1.99	0.62
3:Z:81:PRO:C	3:Z:83:ASP:H	2.03	0.62
3:L:190:LYS:HE2	3:L:210:ASN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:THR:HG22	1:D:269:ALA:HB2	1.81	0.61
2:Y:88:ARG:O	2:Y:118:VAL:HG21	2.00	0.61
2:U:171:HIS:HE1	3:V:138:ASN:ND2	1.98	0.61
3:V:136:LEU:HD21	3:V:196:VAL:HG11	1.82	0.61
3:Z:48:LEU:HB3	3:Z:49:ILE:HD12	1.81	0.61
3:N:108:ARG:NH1	3:N:109:THR:O	2.34	0.61
1:A:204:THR:HA	1:A:231:TYR:O	2.01	0.61
3:V:186:TYR:HA	3:V:192:TYR:OH	2.00	0.60
2:Y:38:VAL:HG22	2:Y:48:TRP:HA	1.81	0.60
3:V:62:ARG:HB2	3:V:77:SER:O	2.01	0.60
1:D:218:GLU:OE2	1:E:252:GLN:HA	2.01	0.60
3:V:112:ALA:HB1	3:V:201:LEU:HD23	1.83	0.60
2:Y:13:VAL:O	2:Y:118:VAL:HA	2.01	0.60
2:Y:14:GLN:OE1	2:Y:119:SER:O	2.20	0.60
2:Y:68:ARG:NH2	2:Y:91:ASP:OD2	2.35	0.60
1:D:279:ARG:NH2	2:U:32:THR:O	2.27	0.60
1:E:207:PRO:HG2	1:E:284:MET:SD	2.42	0.60
3:Z:187:GLU:OE1	3:Z:211:ARG:NH1	2.34	0.60
3:X:108:ARG:NH1	3:X:109:THR:O	2.35	0.59
3:V:193:ALA:HA	3:V:208:SER:OG	2.01	0.59
2:U:150:LYS:NZ	2:U:151:ASP:OD2	2.34	0.59
2:I:133:PRO:HG3	2:I:145:LEU:HB3	1.84	0.59
1:A:207:PRO:HG2	1:A:284:MET:SD	2.42	0.59
3:V:143:GLU:CD	3:V:143:GLU:H	2.04	0.59
1:A:237:LEU:HD13	1:A:284:MET:HG3	1.85	0.58
3:N:187:GLU:OE2	3:N:211:ARG:HD2	2.04	0.58
1:D:210:ASN:HB2	1:D:226:ARG:HG3	1.86	0.58
3:N:142:ARG:HH12	3:N:163:VAL:CG1	2.16	0.58
2:Y:23:CYS:HB3	2:Y:80:LEU:HB3	1.85	0.58
2:U:126:PRO:HB3	2:U:152:TYR:HB3	1.86	0.58
3:N:108:ARG:HG3	3:N:108:ARG:HH11	1.69	0.57
3:X:14:SER:OG	3:X:17:GLU:OE2	2.21	0.57
1:D:216:ALA:HB1	1:D:274:ARG:HH21	1.68	0.57
5:B:402:EDO:O1	1:F:274:ARG:NH2	2.37	0.57
3:V:141:PRO:HB2	3:V:143:GLU:OE2	2.05	0.57
3:M:119:PRO:HB3	3:M:209:PHE:CE1	2.40	0.57
2:Y:133:PRO:HD3	2:Y:145:LEU:HB3	1.84	0.57
2:J:27:GLY:N	1:E:278:GLN:HE22	1.91	0.57
1:E:231:TYR:CD1	1:E:232:PRO:HA	2.40	0.57
2:W:196:LEU:HD12	2:W:220:PRO:HG3	1.85	0.57
2:Y:32:THR:HG22	2:Y:33:TYR:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:173:PHE:CE1	3:Z:164:THR:HG23	2.40	0.57
2:Y:193:SER:HA	2:Y:196:LEU:HD22	1.87	0.57
3:Z:80:GLU:O	3:Z:83:ASP:HB2	2.04	0.56
3:Z:120:PRO:HD3	3:Z:132:VAL:HG22	1.87	0.56
3:Z:71:ASP:OD2	3:Z:71:ASP:N	2.37	0.56
1:F:278:GLN:OE1	6:F:501:HOH:O	2.18	0.56
2:U:32:THR:HG21	5:U:301:EDO:H22	1.88	0.56
2:U:171:HIS:CE1	3:V:138:ASN:HD21	2.22	0.56
1:B:208:MET:HE3	1:B:210:ASN:HD22	1.70	0.56
3:M:149:LYS:HE3	3:M:154:LEU:HD13	1.88	0.56
2:W:123:THR:O	2:W:124:LYS:HD2	2.05	0.56
3:Z:155:GLN:HG2	3:Z:158:ASN:HD21	1.70	0.56
3:M:145:LYS:CE	3:M:147:GLN:HG3	2.30	0.55
3:Z:108:ARG:HG2	3:Z:109:THR:N	2.21	0.55
3:Z:126:LYS:HG3	3:Z:183:LYS:HZ2	1.71	0.55
3:M:179:LEU:HG	3:M:181:LEU:CD2	2.37	0.55
3:M:118:PHE:HB2	3:M:133:VAL:HG22	1.88	0.55
3:L:197:THR:HG22	3:L:204:PRO:HG3	1.87	0.55
3:Z:142:ARG:O	3:Z:142:ARG:NH1	2.39	0.55
3:Z:136:LEU:HD13	3:Z:175:LEU:HD22	1.88	0.55
3:Z:108:ARG:CZ	3:Z:170:ASP:O	2.55	0.55
3:Z:108:ARG:NH1	3:Z:172:THR:CG2	2.65	0.55
5:B:402:EDO:H22	1:F:219:GLY:HA2	1.89	0.54
3:X:122:ASP:N	6:X:301:HOH:O	2.36	0.54
2:Y:3:VAL:HA	2:Y:26:SER:O	2.07	0.54
2:H:13:VAL:HG21	2:H:19:LEU:HD22	1.88	0.54
2:Y:87:LEU:HB3	2:Y:118:VAL:HG11	1.90	0.54
3:L:190:LYS:CE	3:L:211:ARG:N	2.71	0.54
3:M:41:PRO:HG3	3:M:165:GLU:HG2	1.90	0.54
3:V:151:ASP:OD2	3:V:189:HIS:ND1	2.33	0.54
2:W:32:THR:HG22	2:W:33:TYR:CD1	2.43	0.54
3:M:81:PRO:HA	3:M:106:ILE:HG13	1.88	0.54
3:V:140:TYR:CG	3:V:141:PRO:HA	2.43	0.54
1:F:233:ARG:HG3	1:F:264:TYR:CZ	2.43	0.54
2:W:216:LYS:NZ	3:X:123:GLU:OE1	2.28	0.53
1:E:204:THR:N	6:E:501:HOH:O	2.41	0.53
3:Z:62:ARG:HH12	3:Z:83:ASP:CG	2.11	0.53
2:W:8:SER:HA	2:W:114:THR:HG21	1.90	0.53
3:L:190:LYS:HE3	3:L:211:ARG:O	2.09	0.53
3:Z:170:ASP:OD1	3:Z:172:THR:OG1	2.22	0.53
3:V:126:LYS:HG3	3:V:126:LYS:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:5:THR:OG1	3:N:24:ARG:HD3	2.09	0.52
1:D:259:ASP:OD2	1:D:263:THR:OG1	2.27	0.52
3:V:138:ASN:N	3:V:138:ASN:HD22	2.08	0.52
1:F:237:LEU:O	1:F:253:TRP:HZ3	1.93	0.52
3:Z:12:SER:HA	3:Z:105:ASP:HB2	1.91	0.52
3:N:15:PRO:HD3	3:N:106:ILE:HD11	1.90	0.52
1:F:213:ARG:HB3	1:F:221:ILE:HD11	1.91	0.52
3:L:190:LYS:HE3	3:L:211:ARG:CB	2.40	0.52
1:C:292:THR:HG22	6:C:409:HOH:O	2.09	0.52
3:X:62:ARG:HB2	3:X:77:SER:O	2.09	0.52
3:L:145:LYS:HB3	3:L:197:THR:OG1	2.10	0.52
1:A:274:ARG:NH2	5:E:402:EDO:O1	2.43	0.52
1:E:219:GLY:HA2	5:E:402:EDO:C1	2.39	0.52
3:Z:108:ARG:HH21	3:Z:108:ARG:HG3	1.75	0.52
1:E:283:TYR:HD1	1:E:292:THR:HG22	1.74	0.52
2:Y:69:PHE:CE1	2:Y:84:MET:HG2	2.45	0.52
2:H:77:ARG:HD2	2:U:74:ASP:OD2	2.10	0.51
3:X:40:LYS:HB3	3:X:41:PRO:HD2	1.92	0.51
3:M:179:LEU:HG	3:M:181:LEU:HD21	1.92	0.51
3:V:175:LEU:HD23	3:V:176:SER:N	2.24	0.51
3:V:55:ARG:HG2	3:V:59:ILE:HB	1.93	0.51
2:Y:7:GLU:OE1	2:Y:112:GLN:HB2	2.10	0.51
2:Y:94:VAL:CG1	2:Y:113:GLY:HA3	2.41	0.51
2:Y:173:PHE:CE2	3:Z:176:SER:HB3	2.46	0.51
2:H:13:VAL:CG2	2:H:19:LEU:HD22	2.41	0.51
3:V:67:GLY:HA3	3:V:72:PHE:HA	1.93	0.51
3:V:170:ASP:OD1	3:V:172:THR:HG22	2.11	0.51
2:W:217:ARG:H	2:W:217:ARG:NE	2.09	0.51
1:A:236:ILE:HB	1:A:285:GLU:HB2	1.93	0.51
3:V:134:CYS:HB2	3:V:148:TRP:CH2	2.46	0.51
1:C:281:THR:HB	1:C:292:THR:HG23	1.93	0.50
3:N:147:GLN:HG2	3:N:154:LEU:HD11	1.92	0.50
1:D:210:ASN:HB2	1:D:226:ARG:NE	2.26	0.50
2:Y:204:ASN:ND2	2:Y:215:ASP:OD2	2.33	0.50
1:A:273:CYS:O	1:A:276:GLU:HG2	2.11	0.50
1:D:274:ARG:HD3	2:Y:77:ARG:CZ	2.41	0.50
2:U:217:ARG:HD3	2:U:219:GLU:CD	2.31	0.50
3:N:146:VAL:HG22	3:N:196:VAL:HG22	1.93	0.50
1:F:237:LEU:CD1	1:F:284:MET:HG3	2.42	0.50
1:B:219:GLY:HA2	5:B:402:EDO:C1	2.41	0.50
3:Z:13:LEU:HD12	3:Z:17:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:CYS:O	1:D:276:GLU:HG2	2.12	0.50
2:W:202:ILE:HD13	2:W:217:ARG:HA	1.93	0.50
1:D:274:ARG:HD3	2:Y:77:ARG:NH1	2.27	0.50
3:V:175:LEU:HD23	3:V:176:SER:C	2.33	0.50
3:Z:150:VAL:CG1	3:Z:155:GLN:NE2	2.73	0.50
3:L:143:GLU:OE1	3:L:143:GLU:N	2.39	0.49
3:Z:38:GLN:HB2	3:Z:48:LEU:HD21	1.93	0.49
3:M:126:LYS:O	3:M:126:LYS:HD3	2.12	0.49
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.94	0.49
3:V:197:THR:HG22	3:V:204:PRO:HG3	1.93	0.49
1:B:274:ARG:HH21	5:B:402:EDO:C1	2.26	0.49
2:Y:133:PRO:HD3	2:Y:145:LEU:CB	2.42	0.49
3:Z:14:SER:N	3:Z:17:GLU:OE2	2.44	0.49
2:Y:185:LEU:HD23	2:Y:186:SER:N	2.28	0.49
3:L:169:LYS:CE	3:L:170:ASP:HB3	2.43	0.49
3:V:136:LEU:HD21	3:V:196:VAL:CG1	2.42	0.49
3:V:184:ALA:C	3:V:187:GLU:HB2	2.32	0.49
2:Y:159:VAL:HA	2:Y:204:ASN:O	2.13	0.49
2:J:27:GLY:H	1:E:278:GLN:NE2	1.93	0.48
3:N:24:ARG:HA	3:N:70:THR:O	2.13	0.48
1:A:213:ARG:NH1	1:A:277:GLU:OE2	2.45	0.48
2:H:123:THR:HG22	2:H:210:SER:HB3	1.96	0.48
3:Z:62:ARG:NH1	3:Z:83:ASP:OD2	2.47	0.48
1:C:218:GLU:OE1	1:C:271:ARG:NH1	2.44	0.48
1:D:263:THR:O	1:D:264:TYR:HD1	1.96	0.48
1:A:237:LEU:CD1	1:A:284:MET:HG3	2.43	0.48
2:I:132:ALA:HB2	3:M:119:PRO:HD2	1.96	0.48
1:D:242:ASP:OD1	1:D:279:ARG:HD3	2.13	0.48
3:L:81:PRO:HA	3:L:106:ILE:HG13	1.96	0.48
1:F:236:ILE:HB	1:F:285:GLU:HB2	1.95	0.48
1:D:274:ARG:HD3	2:Y:77:ARG:NH2	2.29	0.48
3:M:1:GLU:HG3	3:M:2:ILE:H	1.79	0.48
3:X:119:PRO:HB3	3:X:209:PHE:CE2	2.49	0.48
1:B:208:MET:HE3	1:B:210:ASN:ND2	2.29	0.47
1:B:272:ILE:HD11	1:B:277:GLU:HG3	1.96	0.47
1:D:259:ASP:HB3	1:D:261:ASN:H	1.80	0.47
2:Y:39:ARG:NE	2:Y:47:GLU:OE1	2.45	0.47
3:L:95:SER:H	5:L:301:EDO:H12	1.79	0.47
3:X:197:THR:HG22	3:X:204:PRO:HB3	1.96	0.47
3:Z:108:ARG:HH11	3:Z:172:THR:HA	1.78	0.47
2:H:126:PRO:HB3	2:H:152:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:LEU:HD21	2:H:189:VAL:HG21	1.95	0.47
3:L:78:ARG:HH11	3:L:78:ARG:HD3	1.35	0.47
3:L:190:LYS:HD2	3:L:190:LYS:HA	1.32	0.47
2:Y:65:VAL:HG13	2:Y:69:PHE:HB2	1.97	0.47
3:N:197:THR:HG22	3:N:204:PRO:HG3	1.95	0.47
2:W:191:VAL:HG21	2:W:201:TYR:CZ	2.50	0.47
2:Y:69:PHE:CZ	2:Y:84:MET:HG2	2.50	0.47
3:V:143:GLU:CD	3:V:143:GLU:N	2.66	0.47
2:H:84:MET:HE1	2:H:116:VAL:HG21	1.97	0.47
2:U:216:LYS:HD3	2:U:216:LYS:HA	1.67	0.47
1:E:237:LEU:O	1:E:253:TRP:HZ3	1.97	0.47
1:E:296:PRO:O	1:E:297:SER:HB3	2.15	0.47
2:Y:129:PHE:CG	3:Z:124:GLN:HB2	2.50	0.47
3:N:119:PRO:HB3	3:N:209:PHE:CE1	2.50	0.46
3:V:185:ASP:OD2	3:V:185:ASP:N	2.47	0.46
2:H:5:LEU:O	2:H:112:GLN:OE1	2.32	0.46
2:H:37:TRP:NE1	2:H:82:LEU:HB2	2.30	0.46
2:H:211:ASN:OD1	2:U:14:GLN:HG2	2.14	0.46
2:W:29:THR:O	2:W:32:THR:HB	2.15	0.46
2:W:85:ASN:HD22	2:Y:85:ASN:HD22	1.64	0.46
1:C:259:ASP:HB3	1:C:261:ASN:H	1.80	0.46
2:Y:14:GLN:H	2:Y:14:GLN:HG2	1.52	0.46
3:M:46:ARG:HD3	6:M:302:HOH:O	2.16	0.46
3:V:142:ARG:HB2	3:V:173:TYR:CE1	2.51	0.46
2:H:41:ALA:O	2:H:44:LYS:HB2	2.15	0.46
3:N:5:THR:OG1	3:N:24:ARG:CD	2.64	0.46
1:F:233:ARG:HG3	1:F:264:TYR:CE2	2.51	0.46
3:M:148:TRP:CE3	3:M:179:LEU:HD22	2.51	0.46
1:C:220:ASN:HD22	1:C:271:ARG:NH2	2.09	0.46
3:N:169:LYS:HG3	3:N:170:ASP:H	1.80	0.46
2:Y:169:GLY:O	2:Y:189:VAL:HA	2.15	0.46
3:L:147:GLN:OE1	3:L:154:LEU:HD11	2.16	0.46
3:V:149:LYS:HG2	3:V:154:LEU:HA	1.98	0.46
2:W:208:LYS:HB2	2:W:209:PRO:HD3	1.98	0.46
3:X:190:LYS:HE2	3:X:210:ASN:HB3	1.98	0.46
2:Y:64:SER:O	2:Y:68:ARG:NH1	2.49	0.45
2:Y:178:GLN:HA	3:Z:160:GLN:HE22	1.81	0.45
3:Z:134:CYS:O	3:Z:176:SER:HA	2.16	0.45
3:N:117:ILE:HD12	3:N:194:CYS:HB2	1.99	0.45
2:W:178:GLN:NE2	2:W:184:SER:HB2	2.32	0.45
3:Z:140:TYR:CD1	3:Z:141:PRO:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HG3	1:A:267:TRP:HB3	1.99	0.45
3:L:55:ARG:HD3	3:L:60:PRO:O	2.17	0.45
1:E:219:GLY:CA	5:E:402:EDO:H11	2.44	0.45
2:I:191:VAL:HG22	2:I:192:PRO:HD2	1.99	0.45
1:F:207:PRO:HG2	1:F:284:MET:SD	2.56	0.45
3:L:142:ARG:HE	3:L:142:ARG:HB3	1.58	0.45
1:C:231:TYR:CD1	1:C:232:PRO:HA	2.52	0.45
1:C:259:ASP:HB2	1:C:263:THR:O	2.17	0.45
3:N:194:CYS:O	3:N:206:THR:HA	2.17	0.45
3:Z:136:LEU:HB2	3:Z:175:LEU:HB3	1.97	0.45
3:M:34:LEU:HG	3:M:72:PHE:CD2	2.51	0.45
3:Z:149:LYS:NZ	3:Z:154:LEU:HD22	2.32	0.45
2:Y:19:LEU:O	2:Y:84:MET:HB2	2.17	0.45
2:Y:21:LEU:HD22	2:Y:114:THR:HG21	1.98	0.45
2:Y:32:THR:HG22	2:Y:33:TYR:CE1	2.52	0.45
2:I:95:TYR:O	2:I:113:GLY:HA2	2.17	0.44
3:N:84:PHE:HA	3:N:104:VAL:O	2.17	0.44
3:Z:86:VAL:HA	3:Z:102:THR:O	2.18	0.44
3:V:113:PRO:HD2	3:V:201:LEU:HD21	1.98	0.44
2:Y:149:VAL:HG23	2:Y:149:VAL:O	2.18	0.44
3:L:124:GLN:HG2	3:L:129:THR:O	2.18	0.44
2:W:2:GLU:O	2:W:27:GLY:HA3	2.16	0.44
2:W:13:VAL:HG11	2:W:87:LEU:HD13	1.99	0.44
2:W:32:THR:HG22	2:W:33:TYR:CE1	2.52	0.44
3:N:142:ARG:HB2	3:N:173:TYR:CE2	2.53	0.44
2:Y:96:TYR:CE1	2:Y:112:GLN:O	2.58	0.44
2:J:126:PRO:HB3	2:J:152:TYR:HB3	2.00	0.44
2:W:196:LEU:HA	2:W:196:LEU:HD22	1.84	0.44
3:X:46:ARG:HH21	3:X:46:ARG:HD2	1.56	0.44
3:M:1:GLU:CG	3:M:2:ILE:N	2.80	0.44
3:V:122:ASP:HA	3:V:125:LEU:HD12	2.00	0.44
3:Z:106:ILE:HB	3:Z:166:GLN:NE2	2.32	0.44
3:X:108:ARG:NE	3:X:170:ASP:O	2.44	0.43
3:Z:175:LEU:HD23	3:Z:176:SER:N	2.33	0.43
1:E:282:CYS:O	1:E:292:THR:HA	2.18	0.43
2:Y:146:GLY:HA2	2:Y:161:TRP:CZ2	2.53	0.43
2:U:217:ARG:HD3	2:U:219:GLU:OE2	2.17	0.43
3:Z:48:LEU:C	3:Z:49:ILE:HD12	2.39	0.43
3:L:212:GLY:O	3:L:213:GLU:HG3	2.19	0.43
1:B:206:PRO:HA	1:B:207:PRO:HD3	1.92	0.43
3:V:91:GLN:OE1	3:V:93:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:14:GLN:NE2	2:W:120:SER:HA	2.34	0.43
2:Y:39:ARG:NH2	2:Y:47:GLU:OE1	2.48	0.43
2:Y:173:PHE:O	2:Y:185:LEU:HG	2.19	0.43
3:Z:14:SER:OG	3:Z:107:LYS:HB3	2.18	0.43
3:L:159:SER:HA	3:L:178:THR:O	2.19	0.43
2:J:54:TYR:HA	2:J:73:ARG:NH1	2.33	0.43
3:X:124:GLN:HG2	3:X:129:THR:O	2.19	0.43
3:M:143:GLU:O	3:M:198:HIS:HD2	2.02	0.43
3:M:185:ASP:OD1	3:M:185:ASP:N	2.52	0.43
1:C:259:ASP:HB2	1:C:263:THR:C	2.39	0.43
3:Z:149:LYS:CG	3:Z:154:LEU:HD11	2.43	0.43
3:M:41:PRO:CG	3:M:165:GLU:HG2	2.47	0.43
2:H:199:GLN:OE1	2:H:199:GLN:HA	2.17	0.43
2:U:10:GLY:H	2:U:114:THR:HG21	1.84	0.42
2:I:84:MET:HE1	2:I:116:VAL:HG21	2.01	0.42
3:N:62:ARG:NH1	3:N:80:GLU:HG3	2.34	0.42
3:Z:150:VAL:HA	3:Z:191:VAL:O	2.18	0.42
2:H:34:SER:OG	2:H:53:SER:HA	2.19	0.42
3:X:145:LYS:HB3	3:X:197:THR:OG1	2.19	0.42
2:H:37:TRP:CE2	2:H:82:LEU:HB2	2.54	0.42
2:I:124:LYS:HE2	2:I:151:ASP:O	2.19	0.42
3:Z:164:THR:OG1	3:Z:174:SER:N	2.50	0.42
2:I:216:LYS:HD3	2:I:216:LYS:HA	1.72	0.42
3:M:132:VAL:HG12	3:M:179:LEU:HB3	2.01	0.42
1:E:284:MET:O	1:E:290:HIS:HA	2.20	0.42
1:A:233:ARG:HB3	1:A:264:TYR:CZ	2.55	0.42
3:L:169:LYS:HE3	3:L:170:ASP:HB3	2.00	0.42
3:V:63:PHE:HE1	3:V:76:ILE:HD13	1.84	0.42
3:L:34:LEU:HD22	3:L:72:PHE:CG	2.54	0.42
2:U:110:TRP:CE3	3:V:45:PRO:HD2	2.54	0.42
2:U:213:LYS:HB2	2:U:213:LYS:NZ	2.34	0.42
3:X:124:GLN:HE21	3:X:129:THR:HG23	1.85	0.42
2:Y:7:GLU:OE1	2:Y:7:GLU:N	2.48	0.42
2:I:20:ARG:HG3	2:I:20:ARG:HH11	1.84	0.42
3:M:201:LEU:HD13	3:M:205:VAL:HG23	2.01	0.42
2:Y:68:ARG:O	2:Y:85:ASN:HB2	2.20	0.42
3:Z:11:LEU:HD23	3:Z:11:LEU:HA	1.83	0.42
3:Z:122:ASP:HA	3:Z:125:LEU:HG	2.01	0.42
3:L:190:LYS:HE3	3:L:211:ARG:C	2.39	0.42
5:B:402:EDO:H21	2:U:76:ALA:CB	2.47	0.42
3:Z:140:TYR:O	3:Z:198:HIS:HE1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:LYS:O	3:L:196:VAL:HA	2.20	0.41
2:J:29:THR:O	2:J:32:THR:HB	2.21	0.41
3:L:46:ARG:HD3	6:L:410:HOH:O	2.21	0.41
2:I:55:ARG:HE	2:I:55:ARG:HB2	1.50	0.41
3:M:79:LEU:HD22	3:M:106:ILE:HD11	2.01	0.41
3:N:15:PRO:CD	3:N:106:ILE:HD11	2.49	0.41
1:D:216:ALA:CB	1:D:274:ARG:HH21	2.33	0.41
3:V:113:PRO:HB3	3:V:139:PHE:HB3	2.02	0.41
3:V:125:LEU:O	3:V:183:LYS:HD2	2.20	0.41
1:B:208:MET:CE	1:B:210:ASN:ND2	2.74	0.41
3:X:120:PRO:HD3	3:X:132:VAL:HG22	2.02	0.41
3:M:84:PHE:HB3	3:M:106:ILE:HG12	2.01	0.41
2:U:8:SER:HA	2:U:114:THR:HG21	2.02	0.41
2:U:161:TRP:CZ3	2:U:203:CYS:HB3	2.55	0.41
2:W:159:VAL:HA	2:W:204:ASN:O	2.20	0.41
1:F:237:LEU:O	1:F:253:TRP:CZ3	2.73	0.41
3:L:150:VAL:HG12	3:L:192:TYR:CD2	2.55	0.41
2:U:199:GLN:NE2	2:U:199:GLN:HA	2.35	0.41
3:L:87:TYR:O	3:L:101:GLY:HA2	2.20	0.41
1:D:281:THR:HB	1:D:292:THR:HG23	2.02	0.41
3:V:82:GLU:H	3:V:82:GLU:HG3	0.87	0.41
3:M:106:ILE:HD13	3:M:106:ILE:HA	1.80	0.41
1:E:205:VAL:HG23	1:E:231:TYR:HB3	2.03	0.41
2:Y:21:LEU:HD23	2:Y:21:LEU:HA	1.82	0.41
3:L:91:GLN:OE1	3:L:93:GLY:N	2.53	0.41
1:B:259:ASP:HB3	1:B:261:ASN:H	1.86	0.41
2:H:177:LEU:HD13	2:H:183:TYR:CZ	2.55	0.41
2:U:29:THR:H	5:U:301:EDO:H11	1.85	0.41
3:V:138:ASN:HA	3:V:172:THR:OG1	2.21	0.41
3:Z:126:LYS:HG3	3:Z:183:LYS:HZ1	1.83	0.41
3:Z:182:SER:OG	3:Z:185:ASP:OD1	2.39	0.41
2:I:18:SER:HA	2:I:84:MET:O	2.21	0.41
2:Y:143:ALA:O	2:Y:190:THR:HA	2.21	0.41
3:M:62:ARG:HB2	3:M:77:SER:O	2.21	0.40
3:M:139:PHE:N	3:M:172:THR:OG1	2.54	0.40
1:D:236:ILE:HB	1:D:285:GLU:HB2	2.02	0.40
2:W:191:VAL:HG21	2:W:201:TYR:CE2	2.56	0.40
2:Y:26:SER:HA	6:Y:310:HOH:O	2.21	0.40
3:Z:81:PRO:C	3:Z:83:ASP:N	2.68	0.40
2:Y:154:PRO:HD2	2:Y:209:PRO:HB2	2.03	0.40
2:Y:216:LYS:HG3	2:Y:217:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:62:ARG:NH1	3:V:83:ASP:OD2	2.54	0.40
2:W:34:SER:HB2	2:W:100:TRP:HB3	2.04	0.40
1:F:205:VAL:HA	1:F:206:PRO:HD3	1.95	0.40
1:F:296:PRO:O	1:F:297:SER:OG	2.28	0.40
2:Y:14:GLN:OE1	2:Y:120:SER:HA	2.21	0.40
3:M:203:SER:HB2	3:M:204:PRO:CD	2.44	0.40
1:E:229:SER:HA	1:E:263:THR:HB	2.04	0.40
2:Y:130:PRO:HG3	2:Y:216:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/103 (89%)	90 (98%)	2 (2%)	0	100	100
1	B	93/103 (90%)	92 (99%)	1 (1%)	0	100	100
1	C	91/103 (88%)	89 (98%)	2 (2%)	0	100	100
1	D	91/103 (88%)	89 (98%)	2 (2%)	0	100	100
1	E	92/103 (89%)	90 (98%)	2 (2%)	0	100	100
1	F	92/103 (89%)	90 (98%)	2 (2%)	0	100	100
2	H	209/230 (91%)	205 (98%)	4 (2%)	0	100	100
2	I	207/230 (90%)	200 (97%)	5 (2%)	2 (1%)	15	23
2	J	210/230 (91%)	204 (97%)	6 (3%)	0	100	100
2	U	208/230 (90%)	204 (98%)	4 (2%)	0	100	100
2	W	211/230 (92%)	205 (97%)	6 (3%)	0	100	100
2	Y	213/230 (93%)	203 (95%)	9 (4%)	1 (0%)	29	41
3	L	211/214 (99%)	204 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	211/214 (99%)	200 (95%)	9 (4%)	2 (1%)	17	25
3	N	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	29	41
3	V	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29	41
3	X	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	Z	211/214 (99%)	201 (95%)	6 (3%)	4 (2%)	8	10
All	All	3075/3282 (94%)	2970 (97%)	94 (3%)	11 (0%)	34	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	129	PHE
2	I	132	ALA
3	M	203	SER
3	V	187	GLU
2	Y	112	GLN
3	Z	81	PRO
3	Z	82	GLU
3	Z	110	VAL
3	M	169	LYS
3	Z	109	THR
3	N	211	ARG

### 5.3.2 Protein sidechains [i](#)

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	84/91 (92%)	81 (96%)	3 (4%)	35	54
1	B	85/91 (93%)	81 (95%)	4 (5%)	26	42
1	C	83/91 (91%)	79 (95%)	4 (5%)	25	41
1	D	83/91 (91%)	75 (90%)	8 (10%)	8	12
1	E	84/91 (92%)	79 (94%)	5 (6%)	19	31
1	F	84/91 (92%)	82 (98%)	2 (2%)	49	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	179/192 (93%)	175 (98%)	4 (2%)	52	71
2	I	177/192 (92%)	168 (95%)	9 (5%)	24	39
2	J	179/192 (93%)	174 (97%)	5 (3%)	43	63
2	U	177/192 (92%)	169 (96%)	8 (4%)	27	44
2	W	181/192 (94%)	174 (96%)	7 (4%)	32	50
2	Y	181/192 (94%)	170 (94%)	11 (6%)	18	30
3	L	184/185 (100%)	175 (95%)	9 (5%)	25	40
3	M	184/185 (100%)	170 (92%)	14 (8%)	13	20
3	N	184/185 (100%)	181 (98%)	3 (2%)	62	79
3	V	184/185 (100%)	170 (92%)	14 (8%)	13	20
3	X	184/185 (100%)	177 (96%)	7 (4%)	33	51
3	Z	184/185 (100%)	169 (92%)	15 (8%)	11	17
All	All	2681/2808 (96%)	2549 (95%)	132 (5%)	25	40

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	PRO
1	A	233	ARG
1	A	271	ARG
2	H	135	SER
2	H	145	LEU
2	H	198	THR
2	H	206	ASN
3	L	34	LEU
3	L	57	THR
3	L	126	LYS
3	L	127	SER
3	L	142	ARG
3	L	154	LEU
3	L	169	LYS
3	L	190	LYS
3	L	203	SER
1	B	210	ASN
1	B	217	SER
1	B	247	SER
1	B	271	ARG
2	I	4	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	I	89	ASP
2	I	114	THR
2	I	145	LEU
2	I	168	SER
2	I	185	LEU
2	I	193	SER
2	I	198	THR
2	I	216	LYS
3	M	10	THR
3	M	78	ARG
3	M	105	ASP
3	M	114	SER
3	M	166	GLN
3	M	169	LYS
3	M	170	ASP
3	M	180	THR
3	M	185	ASP
3	M	189	HIS
3	M	194	CYS
3	M	195	GLU
3	M	197	THR
3	M	199	GLN
1	C	226	ARG
1	C	229	SER
1	C	233	ARG
1	C	255	ASP
2	J	13	VAL
2	J	157	VAL
2	J	179	SER
2	J	216	LYS
2	J	217	ARG
3	N	12	SER
3	N	127	SER
3	N	142	ARG
1	D	208	MET
1	D	217	SER
1	D	218	GLU
1	D	229	SER
1	D	233	ARG
1	D	247	SER
1	D	252	GLN
1	D	259	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	U	2	GLU
2	U	18	SER
2	U	22	SER
2	U	114	THR
2	U	168	SER
2	U	179	SER
2	U	204	ASN
2	U	216	LYS
3	V	1	GLU
3	V	14	SER
3	V	61	ASP
3	V	142	ARG
3	V	145	LYS
3	V	154	LEU
3	V	164	THR
3	V	169	LYS
3	V	180	THR
3	V	181	LEU
3	V	185	ASP
3	V	196	VAL
3	V	201	LEU
3	V	207	LYS
1	E	229	SER
1	E	233	ARG
1	E	255	ASP
1	E	263	THR
1	E	271	ARG
2	W	32	THR
2	W	124	LYS
2	W	179	SER
2	W	191	VAL
2	W	199	GLN
2	W	204	ASN
2	W	217	ARG
3	X	11	LEU
3	X	14	SER
3	X	22	SER
3	X	24	ARG
3	X	78	ARG
3	X	114	SER
3	X	127	SER
1	F	249	ASP

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Mol	Chain	Res	Type
1	F	290	HIS
2	Y	32	THR
2	Y	65	VAL
2	Y	117	THR
2	Y	123	THR
2	Y	157	VAL
2	Y	167	THR
2	Y	184	SER
2	Y	196	LEU
2	Y	199	GLN
2	Y	204	ASN
2	Y	213	LYS
3	Z	13	LEU
3	Z	30	SER
3	Z	43	GLN
3	Z	61	ASP
3	Z	71	ASP
3	Z	84	PHE
3	Z	105	ASP
3	Z	108	ARG
3	Z	114	SER
3	Z	123	GLU
3	Z	126	LYS
3	Z	129	THR
3	Z	142	ARG
3	Z	162	SER
3	Z	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	265	GLN
1	A	278	GLN
1	A	290	HIS
2	H	112	GLN
1	B	210	ASN
1	B	290	HIS
2	I	112	GLN
1	C	220	ASN
1	C	265	GLN
3	N	155	GLN

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Mol	Chain	Res	Type
1	D	220	ASN
2	U	78	ASN
2	U	171	HIS
2	U	178	GLN
2	U	199	GLN
3	V	137	ASN
3	V	138	ASN
1	E	278	GLN
1	E	293	HIS
2	W	14	GLN
2	W	83	GLN
1	F	290	HIS
3	Z	6	GLN
3	Z	160	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 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
4	NAG	B	401	1	14,14,15	0.37	0	17,19,21	0.71	0
4	NAG	F	401	1	14,14,15	0.39	0	17,19,21	0.46	0
5	EDO	L	301	-	3,3,3	0.64	0	2,2,2	0.10	0
5	EDO	B	402	-	3,3,3	0.62	0	2,2,2	0.49	0
5	EDO	U	301	-	3,3,3	0.75	0	2,2,2	0.40	0
4	NAG	F	402	1	14,14,15	0.57	0	17,19,21	0.72	0
4	NAG	E	401	1	14,14,15	0.83	1 (7%)	17,19,21	0.76	0
4	NAG	A	401	1	14,14,15	0.84	1 (7%)	17,19,21	0.91	1 (5%)
5	EDO	E	402	-	3,3,3	0.57	0	2,2,2	1.09	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
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
4	NAG	F	401	1	-	1/6/23/26	0/1/1/1
5	EDO	L	301	-	-	0/1/1/1	-
5	EDO	B	402	-	-	0/1/1/1	-
5	EDO	U	301	-	-	1/1/1/1	-
4	NAG	F	402	1	-	0/6/23/26	0/1/1/1
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
5	EDO	E	402	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	NAG	O5-C1	-2.72	1.39	1.43
4	A	401	NAG	O5-C1	2.27	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	NAG	C1-O5-C5	2.06	114.99	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	U	301	EDO	O1-C1-C2-O2
5	E	402	EDO	O1-C1-C2-O2
4	F	401	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	301	EDO	1	0
5	B	402	EDO	7	0
5	U	301	EDO	3	0
5	E	402	EDO	5	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	94/103 (91%)	0.28	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	25, 37, 70, 90	0
1	B	95/103 (92%)	0.26	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 37, 68, 94	0
1	C	93/103 (90%)	0.49	4 (4%) <span style="border: 1px solid red; padding: 2px;">35</span> <span style="border: 1px solid red; padding: 2px;">33</span>	33, 62, 88, 109	0
1	D	93/103 (90%)	1.03	14 (15%) <span style="border: 1px solid red; padding: 2px;">2</span> <span style="border: 1px solid red; padding: 2px;">1</span>	37, 74, 109, 121	0
1	E	94/103 (91%)	0.30	1 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">79</span>	30, 49, 84, 109	0
1	F	94/103 (91%)	0.22	1 (1%) <span style="border: 1px solid blue; padding: 2px;">80</span> <span style="border: 1px solid blue; padding: 2px;">79</span>	29, 49, 92, 107	0
2	H	213/230 (92%)	0.32	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	24, 45, 90, 117	0
2	I	211/230 (91%)	0.34	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	22, 40, 85, 96	0
2	J	214/230 (93%)	0.19	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">89</span>	26, 42, 81, 97	0
2	U	212/230 (92%)	0.35	4 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">64</span>	27, 49, 91, 97	0
2	W	215/230 (93%)	0.23	3 (1%) <span style="border: 1px solid blue; padding: 2px;">75</span> <span style="border: 1px solid blue; padding: 2px;">73</span>	28, 53, 97, 113	0
2	Y	217/230 (94%)	2.04	84 (38%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	32, 79, 140, 155	0
3	L	213/214 (99%)	0.23	4 (1%) <span style="border: 1px solid blue; padding: 2px;">66</span> <span style="border: 1px solid blue; padding: 2px;">64</span>	30, 61, 85, 102	0
3	M	213/214 (99%)	0.58	16 (7%) <span style="border: 1px solid red; padding: 2px;">14</span> <span style="border: 1px solid red; padding: 2px;">13</span>	29, 74, 108, 132	0
3	N	213/214 (99%)	0.25	6 (2%) <span style="border: 1px solid blue; padding: 2px;">53</span> <span style="border: 1px solid blue; padding: 2px;">51</span>	34, 61, 85, 101	0
3	V	213/214 (99%)	1.04	35 (16%) <span style="border: 1px solid red; padding: 2px;">1</span> <span style="border: 1px solid red; padding: 2px;">1</span>	38, 77, 120, 133	0
3	X	213/214 (99%)	0.37	1 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">89</span>	41, 59, 81, 103	0
3	Z	213/214 (99%)	1.80	82 (38%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	54, 102, 143, 162	0
All	All	3123/3282 (95%)	0.61	259 (8%) <span style="border: 1px solid red; padding: 2px;">11</span> <span style="border: 1px solid red; padding: 2px;">10</span>	22, 59, 117, 162	0

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	157	VAL	11.4
2	Y	188	VAL	9.9
3	Z	209	PHE	9.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	140	GLY	8.9
3	V	148	TRP	8.9
2	Y	166	LEU	8.6
2	Y	12	LEU	8.3
3	Z	201	LEU	8.2
2	Y	128	VAL	8.0
3	Z	115	VAL	7.7
2	Y	133	PRO	7.6
2	Y	130	PRO	7.6
2	Y	171	HIS	7.4
2	Y	217	ARG	7.1
2	Y	148	LEU	6.9
2	Y	206	ASN	6.9
2	Y	221	LYS	6.8
3	V	181	LEU	6.6
3	V	154	LEU	6.6
3	Z	119	PRO	6.5
2	Y	134	SER	6.5
2	Y	191	VAL	6.4
2	Y	190	THR	6.2
2	Y	145	LEU	6.1
3	Z	84	PHE	6.0
2	Y	202	ILE	6.0
3	V	209	PHE	5.9
2	Y	159	VAL	5.8
3	V	153	ALA	5.8
3	Z	136	LEU	5.8
3	Z	121	SER	5.7
2	Y	129	PHE	5.7
3	Z	194	CYS	5.7
2	Y	167	THR	5.6
2	Y	135	SER	5.6
3	Z	117	ILE	5.6
2	Y	212	THR	5.5
3	V	194	CYS	5.5
3	V	150	VAL	5.5
3	V	196	VAL	5.5
2	Y	147	CYS	5.5
3	Z	118	PHE	5.3
3	Z	191	VAL	5.3
2	Y	213	LYS	5.2
3	Z	122	ASP	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	220	PRO	5.1
3	Z	210	ASN	5.1
2	Y	132	ALA	5.1
3	V	195	GLU	4.8
2	Y	203	CYS	4.7
2	Y	214	VAL	4.6
2	Y	218	VAL	4.6
2	Y	181	GLY	4.6
3	Z	101	GLY	4.5
3	Z	131	SER	4.5
2	Y	189	VAL	4.5
3	Z	113	PRO	4.5
3	Z	183	LYS	4.4
3	V	132	VAL	4.4
2	Y	205	VAL	4.4
2	Y	141	GLY	4.3
3	V	210	ASN	4.3
3	Z	205	VAL	4.3
3	V	159	SER	4.3
3	Z	85	ALA	4.3
3	Z	139	PHE	4.3
3	V	179	LEU	4.2
2	Y	169	GLY	4.2
3	Z	150	VAL	4.2
3	V	202	SER	4.2
2	Y	196	LEU	4.1
1	D	257	LEU	4.1
2	U	133	PRO	4.1
2	Y	41	ALA	4.0
3	M	1	GLU	4.0
3	Z	204	PRO	4.0
3	Z	125	LEU	4.0
3	V	193	ALA	4.0
3	Z	196	VAL	4.0
3	Z	146	VAL	3.9
2	Y	177	LEU	3.9
3	V	180	THR	3.9
2	Y	182	LEU	3.8
2	Y	146	GLY	3.8
3	Z	110	VAL	3.8
2	W	2	GLU	3.7
1	C	218	GLU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	219	GLU	3.7
2	I	2	GLU	3.7
2	Y	125	GLY	3.7
3	V	206	THR	3.7
2	Y	124	LYS	3.7
2	Y	215	ASP	3.7
1	D	205	VAL	3.6
3	Z	114	SER	3.6
2	Y	207	HIS	3.5
3	Z	202	SER	3.5
3	Z	126	LYS	3.5
1	D	206	PRO	3.5
3	Z	152	ASN	3.5
3	Z	200	GLY	3.5
3	V	147	GLN	3.5
2	Y	94	VAL	3.5
2	Y	131	LEU	3.4
2	Y	193	SER	3.4
1	D	231	TYR	3.4
3	Z	116	PHE	3.4
3	Z	211	ARG	3.4
2	Y	161	TRP	3.4
3	Z	128	GLY	3.4
3	Z	206	THR	3.4
2	Y	116	VAL	3.3
3	Z	173	TYR	3.3
3	Z	192	TYR	3.2
3	V	205	VAL	3.2
3	Z	163	VAL	3.2
2	Y	194	SER	3.2
3	M	202	SER	3.2
2	Y	187	SER	3.2
2	Y	143	ALA	3.2
2	Y	211	ASN	3.2
2	Y	123	THR	3.1
3	Z	4	LEU	3.2
3	X	78	ARG	3.1
3	Z	189	HIS	3.1
3	Z	133	VAL	3.1
3	Z	144	ALA	3.1
2	Y	2	GLU	3.1
3	Z	87	TYR	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	173	PHE	3.1
3	Z	112	ALA	3.1
3	Z	135	LEU	3.1
3	M	78	ARG	3.0
3	V	192	TYR	3.0
2	U	145	LEU	3.0
3	Z	129	THR	3.0
1	D	233	ARG	3.0
1	D	218	GLU	3.0
3	Z	181	LEU	3.0
2	Y	170	VAL	2.9
3	M	150	VAL	2.9
2	Y	175	ALA	2.9
2	Y	13	VAL	2.9
2	Y	186	SER	2.9
2	I	112	GLN	2.9
3	V	1	GLU	2.9
3	M	195	GLU	2.9
2	Y	163	SER	2.8
2	Y	222	SER	2.8
3	M	79	LEU	2.8
3	Z	151	ASP	2.8
2	J	2	GLU	2.8
3	M	196	VAL	2.8
1	D	264	TYR	2.7
3	Z	186	TYR	2.7
2	Y	127	SER	2.7
3	Z	180	THR	2.7
1	D	207	PRO	2.7
1	D	256	VAL	2.7
2	I	218	VAL	2.7
3	M	123	GLU	2.7
2	U	196	LEU	2.7
3	N	142	ARG	2.7
2	Y	151	ASP	2.7
3	N	202	SER	2.7
3	Z	154	LEU	2.7
2	Y	201	TYR	2.6
3	V	191	VAL	2.6
3	Z	12	SER	2.6
1	D	272	ILE	2.6
3	Z	99	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	M	76	ILE	2.6
3	Z	29	VAL	2.6
3	Z	184	ALA	2.6
2	Y	149	VAL	2.6
3	V	133	VAL	2.6
3	Z	106	ILE	2.6
3	V	190	LYS	2.6
3	Z	76	ILE	2.5
3	V	151	ASP	2.5
3	Z	178	THR	2.5
1	C	271	ARG	2.5
2	Y	117	THR	2.5
2	Y	200	THR	2.5
3	N	81	PRO	2.5
3	V	134	CYS	2.5
3	N	199	GLN	2.5
3	Z	105	ASP	2.5
3	Z	98	PHE	2.4
2	Y	198	THR	2.4
3	M	203	SER	2.4
1	E	264	TYR	2.4
3	M	146	VAL	2.4
3	Z	14	SER	2.4
3	Z	190	LYS	2.4
2	Y	122	SER	2.4
3	Z	162	SER	2.4
3	M	205	VAL	2.4
3	Z	107	LYS	2.4
3	V	118	PHE	2.4
3	Z	182	SER	2.4
3	Z	203	SER	2.4
1	D	260	GLY	2.3
2	Y	158	THR	2.3
3	L	168	SER	2.3
3	L	78	ARG	2.3
3	V	112	ALA	2.3
3	Z	212	GLY	2.3
2	Y	154	PRO	2.3
3	N	106	ILE	2.3
2	Y	185	LEU	2.3
3	V	187	GLU	2.3
3	Z	11	LEU	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	Y	112	GLN	2.2
3	L	190	LYS	2.2
3	V	135	LEU	2.2
2	Y	174	PRO	2.2
3	Z	127	SER	2.2
2	Y	92	THR	2.2
3	M	148	TRP	2.2
3	V	158	ASN	2.2
1	C	217	SER	2.2
3	Z	132	VAL	2.2
3	Z	96	PHE	2.2
3	Z	187	GLU	2.2
3	N	196	VAL	2.2
1	D	263	THR	2.2
2	Y	210	SER	2.2
3	V	116	PHE	2.2
3	Z	41	PRO	2.2
3	Z	134	CYS	2.2
1	F	231	TYR	2.2
3	Z	213	GLU	2.2
2	Y	142	THR	2.2
3	M	209	PHE	2.2
2	W	217	ARG	2.1
3	Z	188	LYS	2.1
2	U	144	ALA	2.1
2	Y	156	PRO	2.1
3	M	154	LEU	2.1
3	Z	199	GLN	2.1
3	V	115	VAL	2.1
3	M	11	LEU	2.1
2	Y	195	SER	2.1
3	Z	19	ALA	2.1
3	Z	79	LEU	2.1
3	V	149	LYS	2.1
2	W	218	VAL	2.1
2	Y	14	GLN	2.1
1	D	216	ALA	2.0
3	L	41	PRO	2.0
2	Y	183	TYR	2.0
3	V	161	GLU	2.0
3	Z	149	LYS	2.0
3	Z	130	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	204	THR	2.0
2	Y	3	VAL	2.0
3	Z	143	GLU	2.0
1	C	219	GLY	2.0

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

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

## 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	EDO	U	301	4/4	0.72	0.47	42,42,45,53	0
5	EDO	L	301	4/4	0.82	0.20	46,47,49,51	0
5	EDO	E	402	4/4	0.84	0.34	32,33,34,34	0
4	NAG	F	401	14/15	0.86	0.22	89,96,101,101	0
4	NAG	E	401	14/15	0.92	0.21	57,60,65,65	0
4	NAG	A	401	14/15	0.93	0.16	35,38,45,48	0
4	NAG	B	401	14/15	0.93	0.14	31,39,42,47	0
4	NAG	F	402	14/15	0.93	0.18	59,63,69,73	0
5	EDO	B	402	4/4	0.95	0.34	28,29,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.