



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:11 PM UTC

PDB ID : 7S7I / pdb_00007s7i
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

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>.

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

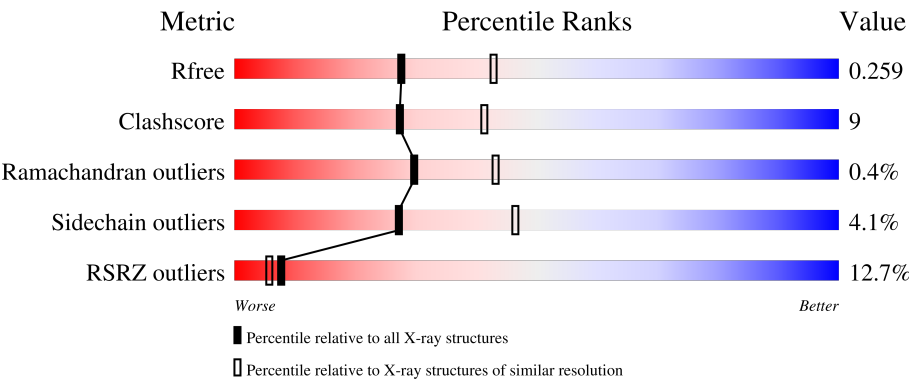
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 ≥ 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	73%18%9%
1	B	103	4% 78%15%8%
1	C	103	10% 75%11%••10%
1	D	103	18% 66%20%••10%
1	E	103	4% 71%18%•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	-

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

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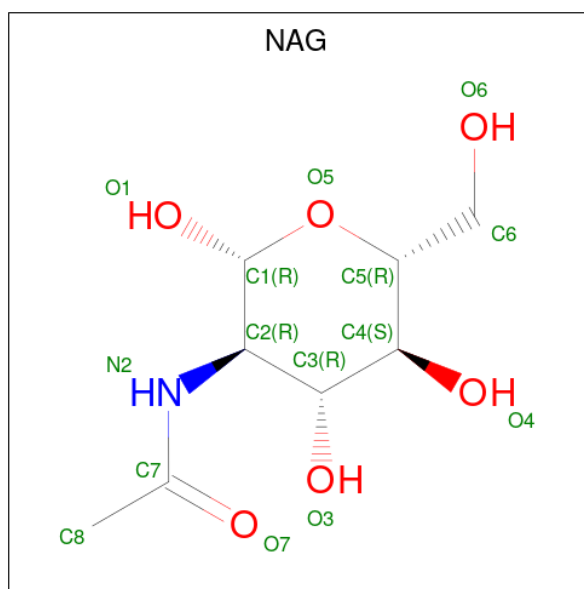
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	215	Total	C	N	O	S	0	0	0
			1633	1032	277	318	6			
2	Y	217	Total	C	N	O	S	0	0	0
			1641	1036	279	320	6			

- 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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



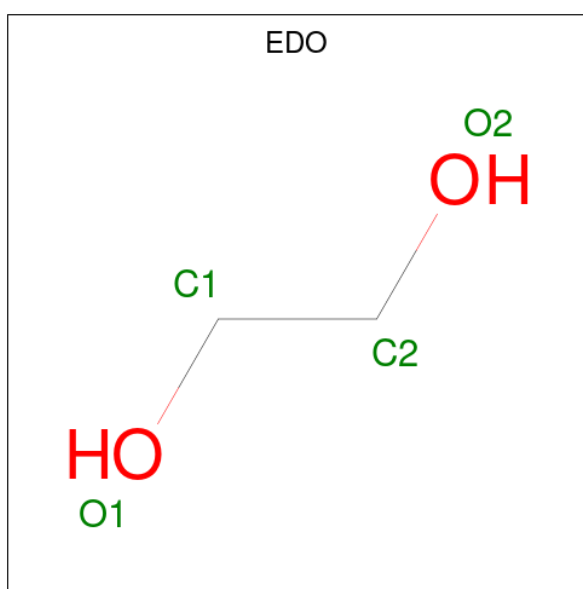
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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 (CCD ID: EDO) (formula: C₂H₆O₂).



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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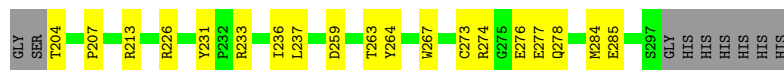
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	58	Total 58	O 58	0	0
6	L	22	Total 22	O 22	0	0
6	B	28	Total 28	O 28	0	0
6	I	54	Total 54	O 54	0	0
6	M	13	Total 13	O 13	0	0
6	C	9	Total 9	O 9	0	0
6	J	52	Total 52	O 52	0	0
6	N	16	Total 16	O 16	0	0
6	D	6	Total 6	O 6	0	0
6	U	31	Total 31	O 31	0	0
6	V	11	Total 11	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.

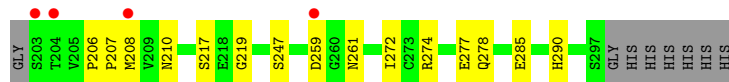
- Molecule 1: MHC class I chain-related protein A

Chain A: 



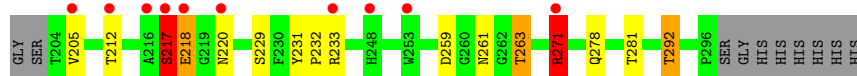
- Molecule 1: MHC class I chain-related protein A

Chain B: 



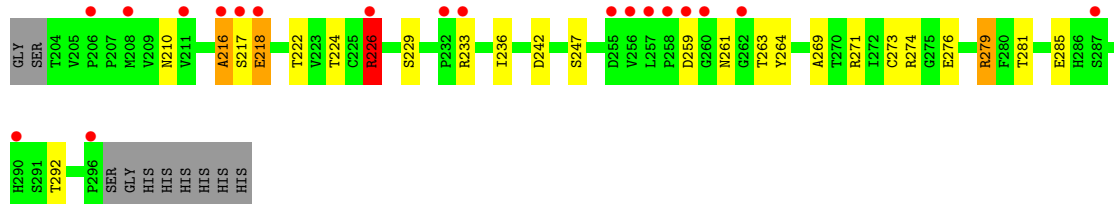
- Molecule 1: MHC class I chain-related protein A

Chain C: 



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

Chain D: 



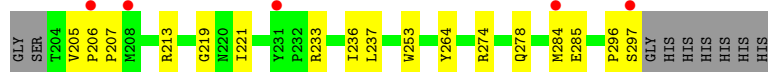
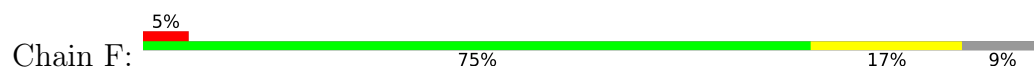
- Molecule 1: MHC class I chain-related protein A

Chain E: 

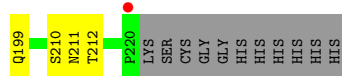
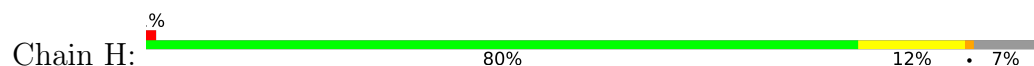




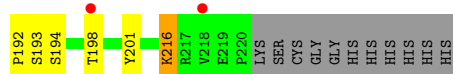
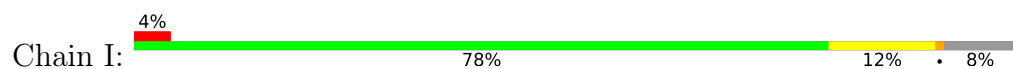
- Molecule 1: MHC class I chain-related protein A



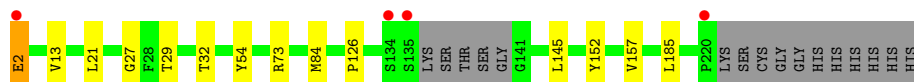
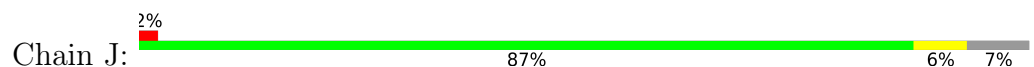
- Molecule 2: Fab heavy chain



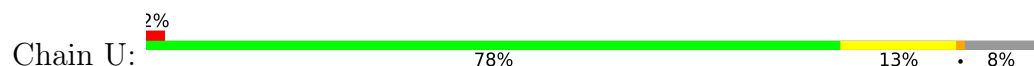
- Molecule 2: Fab heavy chain



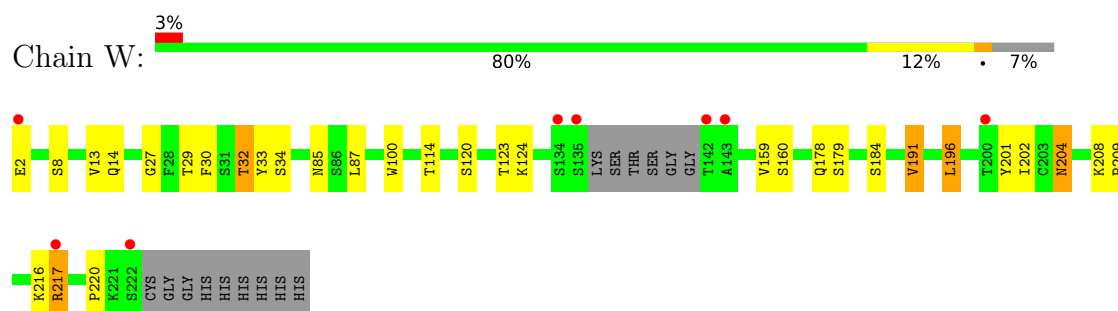
- Molecule 2: Fab heavy chain



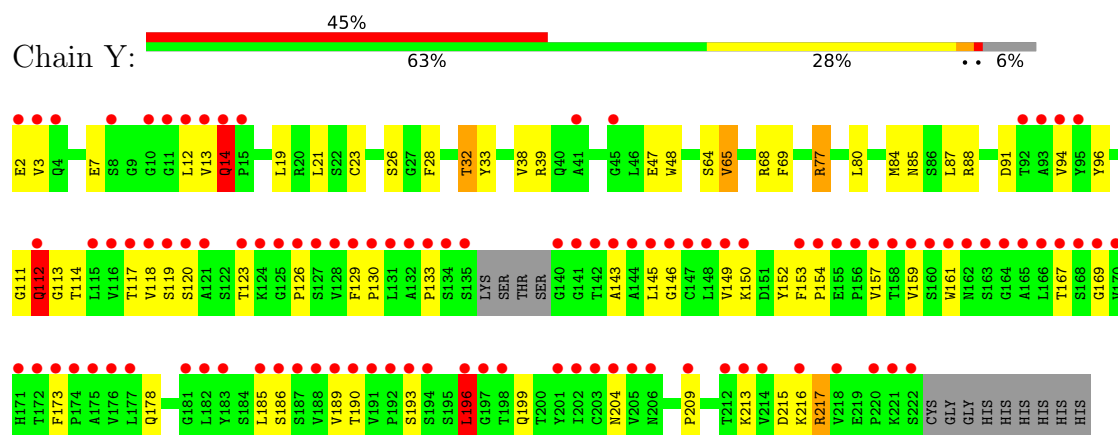
- Molecule 2: Fab heavy chain



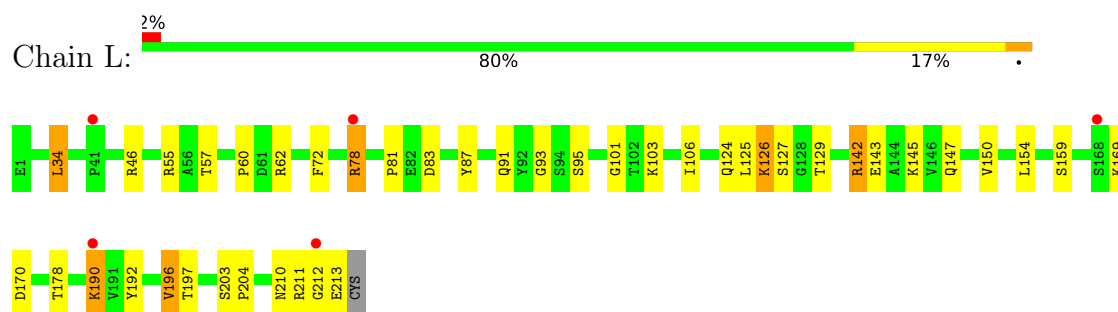
- Molecule 2: Fab heavy chain



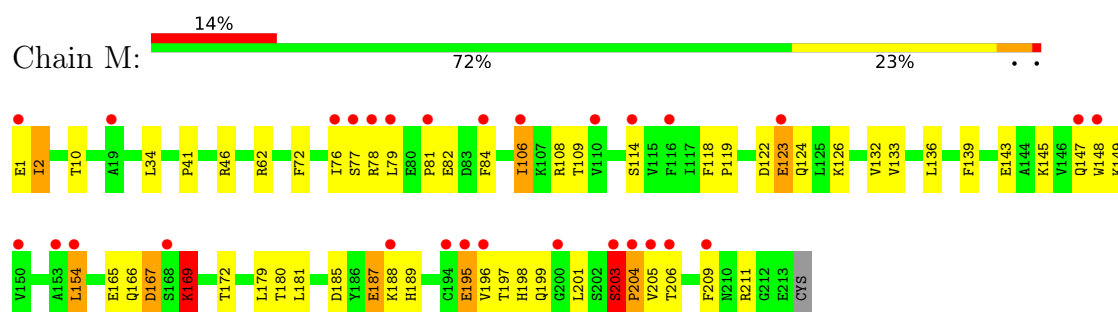
- Molecule 2: Fab heavy chain



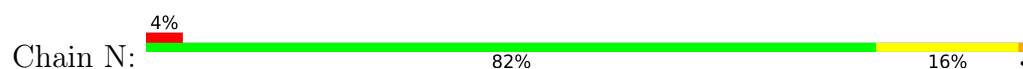
- Molecule 3: Fab light chain

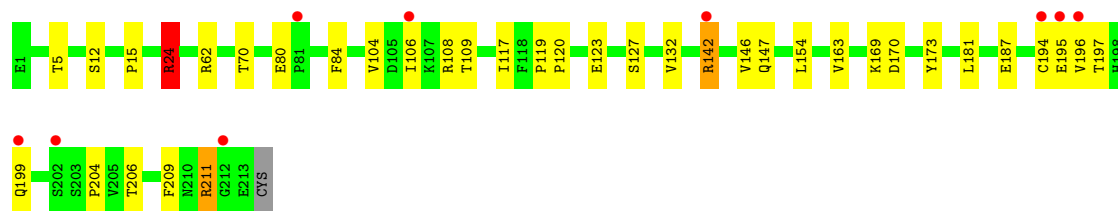


- Molecule 3: Fab light chain

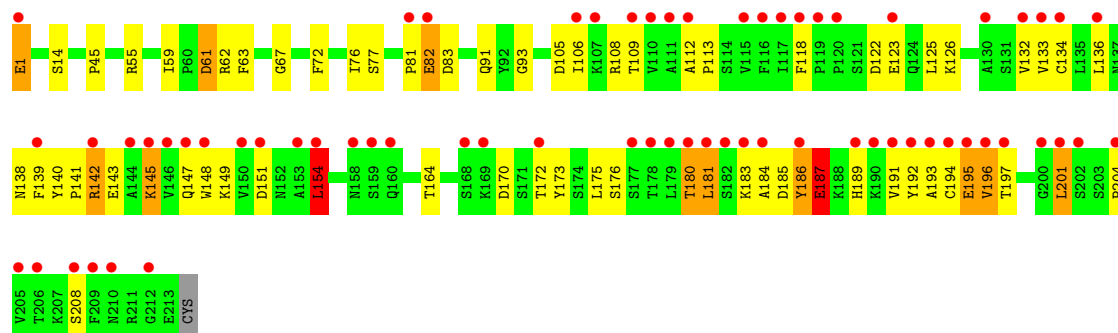


- Molecule 3: Fab light chain

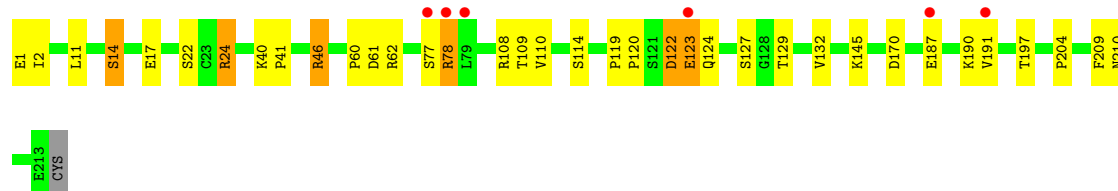
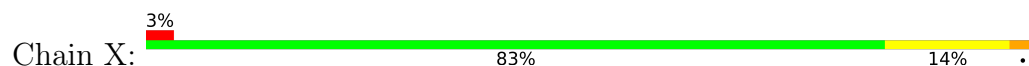




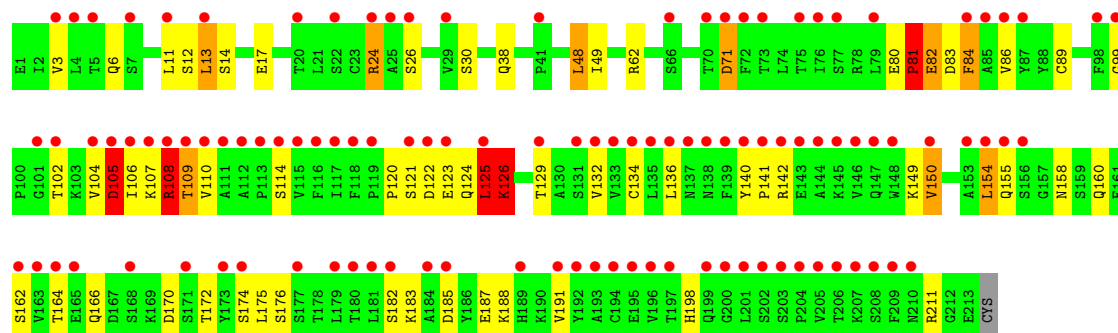
● Molecule 3: Fab light chain



● Molecule 3: Fab light chain



● Molecule 3: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.78Å 170.43Å 148.89Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	44.63 – 2.40 44.63 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.63-2.40) 99.4 (44.63-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.260 0.220 , 0.259	Depositor DCC
R_{free} test set	8731 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24458	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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	0.46	0/761	0.66	0/1040
1	B	0.49	0/767	0.70	0/1048
1	C	0.48	0/755	0.91	7/1032 (0.7%)
1	D	0.42	0/755	0.83	2/1032 (0.2%)
1	E	0.42	0/761	0.63	0/1040
1	F	0.40	0/761	0.59	0/1040
2	H	0.49	0/1659	0.71	3/2260 (0.1%)
2	I	0.51	0/1647	0.85	10/2244 (0.4%)
2	J	0.46	1/1663 (0.1%)	0.64	2/2265 (0.1%)
2	U	0.41	0/1651	0.64	0/2249
2	W	0.40	0/1674	0.73	1/2279 (0.0%)
2	Y	0.49	0/1682	0.99	12/2289 (0.5%)
3	L	0.45	0/1666	0.98	12/2262 (0.5%)
3	M	0.49	0/1666	1.01	11/2262 (0.5%)
3	N	0.45	1/1666 (0.1%)	0.87	8/2262 (0.4%)
3	V	0.56	3/1666 (0.2%)	1.05	18/2262 (0.8%)
3	X	0.45	0/1666	0.92	10/2262 (0.4%)
3	Z	0.50	1/1666 (0.1%)	1.17	16/2262 (0.7%)
All	All	0.47	6/24532 (0.0%)	0.87	112/33390 (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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	V	154	LEU	CG-CD1	8.22	1.79	1.52
3	Z	154	LEU	CG-CD1	-5.96	1.32	1.52
3	V	142	ARG	CB-CG	-5.50	1.35	1.52
2	J	2	GLU	CA-CB	5.36	1.64	1.53
3	N	199	GLN	CD-NE2	5.35	1.44	1.33
3	V	154	LEU	CB-CG	5.14	1.63	1.53

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	154	LEU	CB-CG-CD1	-16.00	62.71	110.70
3	L	78	ARG	CB-CG-CD	-15.80	74.96	111.30
3	L	126	LYS	CB-CA-C	-14.64	85.80	110.68
3	Z	126	LYS	CA-CB-CG	-14.51	85.09	114.10
3	N	24	ARG	CB-CG-CD	-13.70	79.80	111.30
3	L	78	ARG	CA-CB-CG	13.01	140.13	114.10
3	N	142	ARG	CA-CB-CG	12.38	138.86	114.10
2	Y	112	GLN	CA-CB-CG	12.35	138.79	114.10
3	V	123	GLU	CB-CA-C	-12.14	91.61	110.92
3	L	126	LYS	CA-CB-CG	12.06	138.23	114.10
3	X	46	ARG	CB-CG-CD	-12.00	83.69	111.30
3	N	24	ARG	CG-CD-NE	11.28	136.82	112.00
3	Z	24	ARG	CG-CD-NE	11.10	136.41	112.00
3	V	142	ARG	CG-CD-NE	-10.80	88.24	112.00
3	Z	154	LEU	CB-CG-CD2	10.38	141.85	110.70
2	Y	112	GLN	CA-C-N	10.15	141.30	121.41
2	Y	112	GLN	C-N-CA	10.15	141.30	121.41
3	X	123	GLU	N-CA-CB	10.11	124.99	110.12
3	Z	154	LEU	CD1-CG-CD2	-10.11	88.56	110.80
3	X	123	GLU	CA-CB-CG	10.08	134.26	114.10
3	M	154	LEU	CB-CG-CD2	-10.04	80.59	110.70
3	X	46	ARG	CG-CD-NE	9.92	133.82	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	196	LEU	CB-CG-CD2	-9.77	81.39	110.70
3	Z	125	LEU	CA-C-N	-9.23	105.68	122.38
3	Z	125	LEU	C-N-CA	-9.23	105.68	122.38
3	L	78	ARG	CD-NE-CZ	-9.22	111.49	124.40
3	X	24	ARG	CB-CG-CD	8.89	131.74	111.30
3	M	123	GLU	N-CA-CB	8.86	122.86	110.01
3	V	154	LEU	CB-CG-CD2	8.65	136.67	110.70
3	Z	105	ASP	CB-CA-C	-8.55	94.36	110.51
3	M	123	GLU	CB-CA-C	-8.20	98.00	110.88
3	V	142	ARG	CB-CG-CD	7.94	129.56	111.30
3	N	195	GLU	CA-CB-CG	7.91	129.92	114.10
3	V	142	ARG	CA-CB-CG	-7.84	98.43	114.10
3	L	126	LYS	N-CA-CB	7.82	121.78	110.06
3	L	78	ARG	CB-CA-C	-7.80	98.61	112.27
2	I	112	GLN	CA-CB-CG	-7.68	98.73	114.10
1	D	226	ARG	CB-CA-C	-7.68	96.43	109.72
2	I	131	LEU	CA-C-N	7.52	140.15	121.80
2	I	131	LEU	C-N-CA	7.52	140.15	121.80
2	Y	14	GLN	CB-CG-CD	-7.46	99.92	112.60
3	Z	24	ARG	CD-NE-CZ	-7.42	114.02	124.40
3	V	187	GLU	CA-CB-CG	7.39	128.88	114.10
2	Y	196	LEU	CB-CG-CD1	7.29	132.56	110.70
3	X	122	ASP	CA-C-N	-7.25	110.57	120.28
3	X	122	ASP	C-N-CA	-7.25	110.57	120.28
3	V	82	GLU	CA-CB-CG	-7.21	99.68	114.10
3	M	169	LYS	CA-CB-CG	7.14	128.37	114.10
3	Z	105	ASP	N-CA-CB	7.11	121.22	110.42
2	I	132	ALA	C-N-CD	-7.08	95.96	125.00
3	V	154	LEU	N-CA-CB	6.91	119.91	109.34
1	C	217	SER	N-CA-C	-6.91	98.02	108.52
2	Y	77	ARG	CB-CG-CD	6.85	127.05	111.30
3	V	123	GLU	N-CA-CB	6.76	120.10	109.82
1	C	218	GLU	N-CA-CB	-6.75	103.20	114.27
2	H	212	THR	OG1-CB-CG2	6.72	122.75	109.30
2	I	132	ALA	N-CA-C	6.68	124.57	109.81
3	M	122	ASP	CA-C-N	-6.66	111.78	120.44
3	M	122	ASP	C-N-CA	-6.66	111.78	120.44
3	Z	150	VAL	CB-CA-C	6.58	119.54	110.99
3	Z	108	ARG	CG-CD-NE	-6.56	97.56	112.00
3	V	1	GLU	CG-CD-OE2	-6.33	103.83	118.40
3	L	190	LYS	CB-CG-CD	-6.31	96.78	111.30
1	C	271	ARG	CB-CG-CD	6.28	125.75	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	GLU	CA-CB-CG	6.27	126.65	114.10
2	Y	2	GLU	CA-CB-CG	-6.25	101.60	114.10
1	C	271	ARG	N-CA-CB	6.20	120.39	110.16
3	V	195	GLU	CA-CB-CG	6.17	126.43	114.10
2	H	112	GLN	CB-CG-CD	6.15	123.06	112.60
1	C	218	GLU	CA-CB-CG	6.14	126.37	114.10
3	V	154	LEU	CB-CA-C	-6.01	101.36	109.71
2	H	44	LYS	CA-CB-CG	6.01	126.11	114.10
3	M	204	PRO	N-CA-C	5.99	120.91	111.38
2	J	2	GLU	CA-CB-CG	5.96	126.01	114.10
3	X	123	GLU	CB-CA-C	-5.93	100.95	110.79
3	Z	108	ARG	CB-CG-CD	-5.88	97.77	111.30
2	W	196	LEU	CB-CG-CD2	-5.88	93.05	110.70
3	X	78	ARG	CG-CD-NE	5.87	124.92	112.00
3	N	142	ARG	N-CA-CB	-5.87	101.25	110.46
2	Y	2	GLU	CB-CA-C	-5.85	98.99	110.10
3	L	78	ARG	CG-CD-NE	5.83	124.83	112.00
2	I	44	LYS	CB-CG-CD	5.67	124.33	111.30
3	V	123	GLU	CA-CB-CG	5.65	125.39	114.10
3	N	142	ARG	CG-CD-NE	-5.63	99.62	112.00
1	C	217	SER	CA-C-N	-5.62	115.27	125.66
1	C	217	SER	C-N-CA	-5.62	115.27	125.66
3	L	103	LYS	CG-CD-CE	5.50	123.96	111.30
3	N	24	ARG	CA-CB-CG	5.48	125.06	114.10
3	Z	154	LEU	CB-CA-C	5.47	118.78	109.80
3	Z	126	LYS	CB-CG-CD	5.45	123.83	111.30
3	V	61	ASP	N-CA-CB	-5.42	101.96	110.30
3	M	188	LYS	CB-CA-C	-5.41	102.42	111.13
3	Z	82	GLU	CA-CB-CG	5.41	124.91	114.10
3	M	188	LYS	CA-C-N	-5.40	113.36	123.03
3	M	188	LYS	C-N-CA	-5.40	113.36	123.03
3	N	142	ARG	CD-NE-CZ	5.30	131.82	124.40
2	I	44	LYS	CB-CA-C	-5.30	102.31	112.43
2	I	2	GLU	CB-CA-C	5.29	120.16	110.10
2	Y	77	ARG	CA-CB-CG	-5.29	103.53	114.10
2	I	112	GLN	N-CA-C	5.25	119.79	113.17
2	Y	2	GLU	N-CA-C	5.25	125.71	111.00
3	V	1	GLU	CA-CB-CG	5.24	124.57	114.10
3	V	1	GLU	N-CA-C	5.23	125.63	111.00
3	V	123	GLU	N-CA-C	5.17	117.33	111.02
2	J	2	GLU	CB-CG-CD	5.17	121.39	112.60
3	V	145	LYS	CG-CD-CE	5.15	123.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	126	LYS	CB-CG-CD	-5.08	99.62	111.30
1	D	279	ARG	CB-CG-CD	-5.07	99.64	111.30
3	X	61	ASP	N-CA-CB	-5.06	102.55	110.44
3	M	188	LYS	CA-CB-CG	5.05	124.20	114.10
3	L	126	LYS	N-CA-C	-5.04	105.23	111.33
2	Y	217	ARG	CA-CB-CG	5.03	124.16	114.10

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	13	0
1	B	747	0	693	11	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	15	0
2	J	1622	0	1565	8	0
2	U	1610	0	1555	24	0
2	W	1633	0	1580	25	0
2	Y	1641	0	1585	57	0
3	L	1630	0	1581	32	0
3	M	1630	0	1581	37	0
3	N	1630	0	1581	24	0
3	V	1630	0	1581	51	0
3	X	1630	0	1581	16	0
3	Z	1630	0	1581	59	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	16	0	0	1	0
All	All	24458	0	23098	428	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 (428) 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
1:B:208:MET:HE1	1:B:210:ASN:HD22	1.07	1.18
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:B:208:MET:HE1	1:B:210:ASN:ND2	1.82	0.93
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
3:Z:126:LYS:HA	3:Z:183:LYS:HZ2	1.46	0.81
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
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: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
1:B:208:MET:CE	1:B:210:ASN:HD22	1.94	0.75
3:Z:126:LYS:HG3	3:Z:183:LYS:HZ2	1.50	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
3:Z:81:PRO:C	3:Z:83:ASP:H	2.03	0.66
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
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:Z:126:LYS:HG3	3:Z:183:LYS:NZ	2.11	0.64
3:M:1:GLU:HG3	3:M:2:ILE:N	2.12	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
2:I:84:MET:HE1	2:I:116:VAL:HG21	1.80	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:143:GLU:CD	3:V:143:GLU:H	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:U:84:MET:HE1	2:U:116:VAL:HG21	1.81	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:L:190:LYS:HE2	3:L:210:ASN:HB3	1.83	0.61
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
2:W:216:LYS:NZ	3:X:123:GLU:OE1	2.28	0.60
1:D:218:GLU:OE2	1:E:252:GLN:HA	2.01	0.60
2:U:150:LYS:NZ	2:U:151:ASP:OD2	2.34	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Z:62:ARG:HH12	3:Z:83:ASP:CG	2.11	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
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
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: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
2:U:217:ARG:HD3	2:U:219:GLU:CD	2.31	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:V:142:ARG:HG3	3:V:142:ARG:O	1.80	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
3:V:175:LEU:HD23	3:V:176:SER:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:V:184:ALA:C	3:V:187:GLU:HB2	2.32	0.53
1:E:204:THR:N	6:E:501:HOH:O	2.41	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:108:ARG:HG2	3:Z:109:THR:N	2.21	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
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:V:143:GLU:CD	3:V:143:GLU:N	2.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
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
2:H:84:MET:HE1	2:H:116:VAL:HG21	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:ASP:OD1	1:D:279:ARG:HD3	2.13	0.48
3:Z:81:PRO:C	3:Z:83:ASP:N	2.68	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
3:Z:48:LEU:C	3:Z:49:ILE:HD12	2.39	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:272:ILE:HD11	1:B:277:GLU:HG3	1.96	0.47
1:C:259:ASP:HB2	1:C:263:THR:C	2.39	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
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
2:Y:21:LEU:HG	2:Y:84:MET:HE2	1.96	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:L:190:LYS:HE3	3:L:211:ARG:C	2.39	0.46
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:J:21:LEU:HG	2:J:84:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:62:ARG:HH12	3:L:83:ASP:CG	2.20	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
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
1:A:284:MET:HE2	1:A:284:MET:HB3	1.89	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
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:7:GLU:CD	2:I:113:GLY:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:M:82:GLU:H	3:M:82:GLU:CD	2.22	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
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:V:180:THR:C	3:V:181:LEU:HD23	2.46	0.41
3:M:106:ILE:HD13	3:M:106:ILE:HA	1.80	0.41
3:V:151:ASP:CG	3:V:189:HIS:HB3	2.45	0.41
1:E:205:VAL:HG23	1:E:231:TYR:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:123:GLU:O	3:M:124:GLN:C	2.63	0.40
2:W:30:PHE:C	2:W:32:THR:H	2.29	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
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:L:125:LEU:O	3:L:126:LYS:C	2.62	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%)	12	20
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%)	24	37
3	L	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
3	M	211/214 (99%)	200 (95%)	9 (4%)	2 (1%)	14	22
3	N	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	24	37
3	V	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	37
3	X	211/214 (99%)	201 (95%)	10 (5%)	0	100	100
3	Z	211/214 (99%)	201 (95%)	6 (3%)	4 (2%)	6	8
All	All	3075/3282 (94%)	2970 (97%)	94 (3%)	11 (0%)	30	43

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 ⓘ

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%)	84 (100%)	0	100	100
1	B	85/91 (93%)	83 (98%)	2 (2%)	43	65
1	C	83/91 (91%)	78 (94%)	5 (6%)	17	31
1	D	83/91 (91%)	78 (94%)	5 (6%)	17	31
1	E	84/91 (92%)	82 (98%)	2 (2%)	43	65
1	F	84/91 (92%)	84 (100%)	0	100	100
2	H	179/192 (93%)	175 (98%)	4 (2%)	45	67
2	I	177/192 (92%)	169 (96%)	8 (4%)	24	42
2	J	179/192 (93%)	175 (98%)	4 (2%)	45	67
2	U	177/192 (92%)	170 (96%)	7 (4%)	28	47
2	W	181/192 (94%)	176 (97%)	5 (3%)	38	60
2	Y	181/192 (94%)	170 (94%)	11 (6%)	17	30
3	L	184/185 (100%)	179 (97%)	5 (3%)	39	62
3	M	184/185 (100%)	172 (94%)	12 (6%)	15	27
3	N	184/185 (100%)	181 (98%)	3 (2%)	55	76
3	V	184/185 (100%)	170 (92%)	14 (8%)	12	21
3	X	184/185 (100%)	174 (95%)	10 (5%)	20	35
3	Z	184/185 (100%)	171 (93%)	13 (7%)	13	23
All	All	2681/2808 (96%)	2571 (96%)	110 (4%)	27	46

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	135	SER
2	H	157	VAL
2	H	185	LEU
2	H	198	THR
3	L	34	LEU
3	L	57	THR

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Mol	Chain	Res	Type
3	L	127	SER
3	L	196	VAL
3	L	203	SER
1	B	217	SER
1	B	247	SER
2	I	13	VAL
2	I	89	ASP
2	I	114	THR
2	I	185	LEU
2	I	193	SER
2	I	194	SER
2	I	198	THR
2	I	216	LYS
3	M	2	ILE
3	M	10	THR
3	M	76	ILE
3	M	78	ARG
3	M	106	ILE
3	M	114	SER
3	M	166	GLN
3	M	169	LYS
3	M	180	THR
3	M	195	GLU
3	M	197	THR
3	M	199	GLN
1	C	205	VAL
1	C	212	THR
1	C	229	SER
1	C	263	THR
1	C	292	THR
2	J	13	VAL
2	J	145	LEU
2	J	157	VAL
2	J	185	LEU
3	N	12	SER
3	N	127	SER
3	N	181	LEU
1	D	217	SER
1	D	218	GLU
1	D	229	SER
1	D	233	ARG
1	D	247	SER

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Mol	Chain	Res	Type
2	U	2	GLU
2	U	18	SER
2	U	22	SER
2	U	32	THR
2	U	114	THR
2	U	168	SER
2	U	179	SER
3	V	1	GLU
3	V	14	SER
3	V	61	ASP
3	V	105	ASP
3	V	109	THR
3	V	132	VAL
3	V	145	LYS
3	V	154	LEU
3	V	164	THR
3	V	180	THR
3	V	181	LEU
3	V	191	VAL
3	V	196	VAL
3	V	201	LEU
1	E	229	SER
1	E	263	THR
2	W	32	THR
2	W	179	SER
2	W	191	VAL
2	W	204	ASN
2	W	217	ARG
3	X	2	ILE
3	X	11	LEU
3	X	14	SER
3	X	22	SER
3	X	78	ARG
3	X	110	VAL
3	X	114	SER
3	X	127	SER
3	X	187	GLU
3	X	191	VAL
2	Y	14	GLN
2	Y	32	THR
2	Y	65	VAL
2	Y	117	THR

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Mol	Chain	Res	Type
2	Y	123	THR
2	Y	150	LYS
2	Y	157	VAL
2	Y	167	THR
2	Y	196	LEU
2	Y	199	GLN
2	Y	213	LYS
3	Z	13	LEU
3	Z	30	SER
3	Z	48	LEU
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	162	SER
3	Z	188	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	ASN
1	A	241	GLN
1	A	252	GLN
1	A	265	GLN
1	A	278	GLN
1	A	290	HIS
2	H	83	GLN
2	H	112	GLN
2	H	206	ASN
3	L	43	GLN
3	L	160	GLN
3	L	166	GLN
1	B	210	ASN
1	B	248	HIS
1	B	290	HIS
2	I	40	GLN
2	I	112	GLN
3	M	38	GLN

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Mol	Chain	Res	Type
3	M	39	GLN
3	M	43	GLN
3	M	210	ASN
1	C	220	ASN
1	C	265	GLN
1	C	293	HIS
2	J	40	GLN
3	N	39	GLN
3	N	155	GLN
3	N	199	GLN
1	D	220	ASN
1	D	261	ASN
1	D	265	GLN
1	D	290	HIS
1	D	293	HIS
2	U	78	ASN
2	U	171	HIS
2	U	178	GLN
2	U	199	GLN
3	V	137	ASN
3	V	138	ASN
3	V	152	ASN
1	E	278	GLN
2	W	14	GLN
2	W	199	GLN
3	X	27	GLN
3	X	147	GLN
2	Y	171	HIS
3	Z	6	GLN
3	Z	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	F	401	1	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	A	401	1	14,14,15	0.84	1 (7%)	17,19,21	0.92	1 (5%)
4	NAG	F	402	1	14,14,15	0.59	0	17,19,21	0.72	0
5	EDO	L	301	-	3,3,3	0.61	0	2,2,2	0.15	0
5	EDO	B	402	-	3,3,3	0.56	0	2,2,2	0.50	0
5	EDO	E	402	-	3,3,3	0.53	0	2,2,2	1.03	0
4	NAG	E	401	1	14,14,15	0.80	1 (7%)	17,19,21	0.76	0
5	EDO	U	301	-	3,3,3	0.71	0	2,2,2	0.34	0
4	NAG	B	401	1	14,14,15	0.37	0	17,19,21	0.70	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	F	401	1	-	1/6/23/26	0/1/1/1
4	NAG	A	401	1	-	0/6/23/26	0/1/1/1
4	NAG	F	402	1	-	0/6/23/26	0/1/1/1
5	EDO	L	301	-	-	0/1/1/1	-
5	EDO	B	402	-	-	0/1/1/1	-
5	EDO	E	402	-	-	1/1/1/1	-
4	NAG	E	401	1	-	0/6/23/26	0/1/1/1
5	EDO	U	301	-	-	1/1/1/1	-
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	401	NAG	O5-C1	-2.57	1.39	1.43
4	A	401	NAG	O5-C1	2.17	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	2.09	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	E	402	EDO	5	0
5	U	301	EDO	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	94/103 (91%)	-0.18	0 100 100	25, 37, 70, 90	0
1	B	95/103 (92%)	-0.04	4 (4%) 40 36	24, 37, 68, 94	0
1	C	93/103 (90%)	0.67	10 (10%) 11 8	33, 62, 88, 109	0
1	D	93/103 (90%)	1.15	19 (20%) 3 2	37, 74, 109, 121	0
1	E	94/103 (91%)	0.33	4 (4%) 40 36	30, 49, 84, 109	0
1	F	94/103 (91%)	0.45	5 (5%) 32 28	29, 49, 92, 107	0
2	H	213/230 (92%)	0.01	3 (1%) 73 69	24, 45, 90, 117	0
2	I	211/230 (91%)	-0.09	9 (4%) 40 36	22, 40, 85, 96	0
2	J	214/230 (93%)	-0.14	4 (1%) 66 62	26, 42, 81, 97	0
2	U	212/230 (92%)	0.17	4 (1%) 66 62	27, 49, 91, 97	0
2	W	215/230 (93%)	0.35	8 (3%) 45 41	28, 53, 97, 113	0
2	Y	217/230 (94%)	2.01	104 (47%) 0 0	32, 79, 140, 155	0
3	L	213/214 (99%)	0.23	5 (2%) 61 57	30, 61, 85, 102	0
3	M	213/214 (99%)	0.74	29 (13%) 7 5	29, 74, 108, 132	0
3	N	213/214 (99%)	0.40	9 (4%) 40 36	34, 61, 85, 101	0
3	V	213/214 (99%)	1.30	66 (30%) 1 1	38, 77, 120, 133	0
3	X	213/214 (99%)	0.36	6 (2%) 55 51	41, 59, 81, 103	0
3	Z	213/214 (99%)	2.20	109 (51%) 0 0	54, 102, 143, 162	0
All	All	3123/3282 (95%)	0.59	398 (12%) 8 6	22, 59, 117, 162	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	188	VAL	7.3
2	Y	157	VAL	7.0
3	Z	84	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
2	Y	171	HIS	6.2
2	Y	166	LEU	6.1
2	Y	128	VAL	5.7
3	Z	119	PRO	5.7
3	V	195	GLU	5.6
2	Y	168	SER	5.5
3	Z	117	ILE	5.5
2	Y	12	LEU	5.4
2	Y	131	LEU	5.4
3	Z	135	LEU	5.3
3	V	194	CYS	5.3
2	Y	133	PRO	5.2
2	Y	201	TYR	5.2
3	V	148	TRP	5.1
2	Y	145	LEU	5.1
2	Y	148	LEU	5.1
3	Z	115	VAL	5.1
3	V	193	ALA	5.0
2	Y	190	THR	5.0
2	Y	189	VAL	5.0
3	Z	112	ALA	5.0
3	Z	136	LEU	5.0
3	V	153	ALA	4.9
3	V	181	LEU	4.9
2	Y	132	ALA	4.9
3	Z	173	TYR	4.9
2	Y	159	VAL	4.8
3	L	190	LYS	4.8
2	Y	156	PRO	4.7
3	Z	209	PHE	4.7
2	Y	116	VAL	4.6
3	Z	201	LEU	4.6
2	Y	205	VAL	4.6
2	Y	2	GLU	4.6
3	M	1	GLU	4.6
1	F	297	SER	4.6
2	Y	170	VAL	4.5
3	N	199	GLN	4.5
3	V	205	VAL	4.4
2	W	2	GLU	4.4
2	Y	158	THR	4.4
2	Y	177	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
3	V	191	VAL	4.4
2	Y	165	ALA	4.4
3	Z	118	PHE	4.3
2	Y	202	ILE	4.3
3	Z	193	ALA	4.3
3	Z	181	LEU	4.3
3	V	196	VAL	4.2
3	Z	85	ALA	4.2
2	Y	220	PRO	4.2
3	V	197	THR	4.2
3	V	209	PHE	4.2
3	Z	179	LEU	4.1
2	Y	206	ASN	4.1
2	Y	141	GLY	4.1
2	Y	130	PRO	4.0
2	Y	203	CYS	4.0
2	Y	169	GLY	4.0
3	Z	113	PRO	4.0
3	Z	144	ALA	4.0
3	Z	194	CYS	4.0
2	Y	161	TRP	3.9
1	D	218	GLU	3.9
2	I	112	GLN	3.9
2	Y	218	VAL	3.9
2	Y	143	ALA	3.9
2	Y	164	GLY	3.9
3	V	202	SER	3.9
3	V	117	ILE	3.9
2	Y	192	PRO	3.9
2	I	2	GLU	3.8
3	V	204	PRO	3.8
3	V	150	VAL	3.8
3	Z	163	VAL	3.8
3	Z	25	ALA	3.8
2	Y	45	GLY	3.8
2	Y	140	GLY	3.8
3	V	154	LEU	3.8
2	Y	160	SER	3.8
2	Y	175	ALA	3.8
2	Y	174	PRO	3.8
3	M	154	LEU	3.8
3	Z	139	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
3	Z	106	ILE	3.7
3	Z	196	VAL	3.6
3	Z	131	SER	3.6
2	Y	147	CYS	3.6
2	Y	94	VAL	3.6
2	Y	134	SER	3.6
1	D	257	LEU	3.6
2	Y	197	GLY	3.6
3	Z	133	VAL	3.6
2	Y	181	GLY	3.5
3	Z	204	PRO	3.5
3	V	1	GLU	3.5
3	Z	24	ARG	3.5
3	Z	114	SER	3.5
3	Z	116	PHE	3.5
2	Y	191	VAL	3.5
3	Z	109	THR	3.5
3	Z	197	THR	3.5
3	M	153	ALA	3.5
3	Z	200	GLY	3.5
2	Y	129	PHE	3.5
2	Y	155	GLU	3.4
2	Y	14	GLN	3.4
3	V	147	GLN	3.4
3	Z	129	THR	3.4
2	W	142	THR	3.4
2	Y	142	THR	3.4
3	V	110	VAL	3.4
2	J	2	GLU	3.4
3	Z	3	VAL	3.4
3	Z	110	VAL	3.4
3	Z	205	VAL	3.4
2	W	222	SER	3.4
2	Y	194	SER	3.4
2	Y	172	THR	3.3
3	Z	99	GLY	3.3
3	Z	87	TYR	3.3
3	V	179	LEU	3.3
2	Y	149	VAL	3.3
2	Y	167	THR	3.3
3	Z	104	VAL	3.3
3	Z	191	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	Y	187	SER	3.3
3	M	205	VAL	3.3
2	Y	186	SER	3.3
1	F	231	TYR	3.3
2	Y	196	LEU	3.3
2	U	141	GLY	3.3
2	Y	119	SER	3.2
3	Z	13	LEU	3.2
1	C	271	ARG	3.2
2	U	133	PRO	3.2
3	V	192	TYR	3.2
2	Y	212	THR	3.2
3	V	208	SER	3.2
3	Z	101	GLY	3.2
3	V	132	VAL	3.2
2	Y	41	ALA	3.1
3	V	210	ASN	3.1
2	J	135	SER	3.1
3	Z	202	SER	3.1
3	N	142	ARG	3.1
2	Y	112	GLN	3.0
2	Y	221	LYS	3.0
3	V	182	SER	3.0
2	Y	185	LEU	3.0
3	Z	108	ARG	3.0
3	L	212	GLY	3.0
3	V	146	VAL	3.0
1	C	218	GLU	3.0
2	Y	117	THR	3.0
3	L	78	ARG	3.0
3	V	142	ARG	3.0
3	V	190	LYS	3.0
1	D	256	VAL	2.9
3	Z	86	VAL	2.9
3	V	111	ALA	2.9
3	Z	153	ALA	2.9
2	J	220	PRO	2.9
3	Z	155	GLN	2.9
2	H	220	PRO	2.9
3	Z	7	SER	2.9
2	Y	198	THR	2.9
3	V	119	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
3	Z	125	LEU	2.9
3	Z	122	ASP	2.9
3	Z	192	TYR	2.9
3	Z	4	LEU	2.9
3	V	159	SER	2.8
2	Y	3	VAL	2.8
3	Z	132	VAL	2.8
3	Z	150	VAL	2.8
2	Y	154	PRO	2.8
1	C	216	ALA	2.8
1	D	226	ARG	2.8
2	Y	214	VAL	2.8
3	M	196	VAL	2.8
3	X	191	VAL	2.8
3	Z	206	THR	2.8
2	U	144	ALA	2.8
2	W	135	SER	2.8
2	Y	176	VAL	2.8
3	Z	73	THR	2.8
2	H	112	GLN	2.8
3	V	82	GLU	2.8
2	Y	153	PHE	2.8
3	Z	98	PHE	2.8
3	Z	22	SER	2.8
2	Y	10	GLY	2.7
3	Z	174	SER	2.7
3	Z	203	SER	2.7
2	I	132	ALA	2.7
3	V	123	GLU	2.7
3	Z	165	GLU	2.7
3	V	118	PHE	2.7
1	C	205	VAL	2.7
2	Y	135	SER	2.7
3	Z	140	TYR	2.7
3	Z	177	SER	2.7
2	W	200	THR	2.7
3	Z	75	THR	2.7
3	Z	180	THR	2.7
1	D	260	GLY	2.7
3	Z	210	ASN	2.7
2	Y	163	SER	2.7
2	Y	123	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	V	206	THR	2.7
3	V	116	PHE	2.7
3	V	107	LYS	2.7
3	N	202	SER	2.7
3	Z	79	LEU	2.7
2	Y	92	THR	2.7
2	Y	144	ALA	2.7
3	V	130	ALA	2.7
3	Z	105	ASP	2.6
2	Y	173	PHE	2.6
3	Z	142	ARG	2.6
3	Z	154	LEU	2.6
2	Y	150	LYS	2.6
3	M	188	LYS	2.6
3	Z	41	PRO	2.6
3	X	78	ARG	2.6
2	H	135	SER	2.6
2	Y	193	SER	2.6
3	L	168	SER	2.6
3	Z	26	SER	2.6
1	D	258	PRO	2.6
2	Y	182	LEU	2.6
2	Y	13	VAL	2.6
3	V	158	ASN	2.6
3	Z	134	CYS	2.6
2	Y	127	SER	2.6
2	Y	121	ALA	2.6
3	M	79	LEU	2.6
3	M	123	GLU	2.6
2	I	218	VAL	2.6
2	Y	118	VAL	2.6
3	Z	137	ASN	2.6
3	Z	199	GLN	2.6
2	Y	120	SER	2.6
3	M	77	SER	2.6
2	Y	183	TYR	2.6
2	Y	15	PRO	2.5
3	V	106	ILE	2.5
3	Z	123	GLU	2.5
2	Y	204	ASN	2.5
1	D	216	ALA	2.5
3	V	134	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	V	183	LYS	2.5
3	Z	171	SER	2.5
2	Y	11	GLY	2.5
3	X	123	GLU	2.5
3	V	136	LEU	2.5
2	Y	4	GLN	2.5
3	M	110	VAL	2.5
3	Z	207	LYS	2.5
2	W	143	ALA	2.5
2	Y	126	PRO	2.5
2	I	128	VAL	2.5
3	Z	184	ALA	2.5
1	C	217	SER	2.5
3	Z	70	THR	2.5
3	Z	168	SER	2.5
3	Z	208	SER	2.5
3	V	120	PRO	2.5
1	E	260	GLY	2.5
3	Z	138	ASN	2.4
3	V	144	ALA	2.4
3	Z	111	ALA	2.4
1	B	203	SER	2.4
1	D	287	SER	2.4
3	M	148	TRP	2.4
3	Z	146	VAL	2.4
2	U	220	PRO	2.4
1	D	211	VAL	2.4
3	Z	29	VAL	2.4
1	C	220	ASN	2.4
3	V	145	LYS	2.4
3	Z	77	SER	2.4
3	M	150	VAL	2.4
3	Z	145	LYS	2.4
1	D	296	PRO	2.3
3	M	168	SER	2.3
3	Z	156	SER	2.3
2	Y	146	GLY	2.3
3	Z	76	ILE	2.3
3	Z	189	HIS	2.3
1	D	208	MET	2.3
1	F	284	MET	2.3
1	D	206	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	Y	209	PRO	2.3
3	Z	5	THR	2.3
3	Z	20	THR	2.3
1	D	233	ARG	2.3
3	V	201	LEU	2.3
3	M	116	PHE	2.3
3	V	169	LYS	2.3
3	M	195	GLU	2.3
3	V	180	THR	2.3
3	M	203	SER	2.3
3	N	212	GLY	2.3
3	M	76	ILE	2.3
3	X	79	LEU	2.3
3	Z	11	LEU	2.3
2	Y	124	LYS	2.3
3	Z	143	GLU	2.3
2	Y	93	ALA	2.3
2	Y	162	ASN	2.3
3	M	19	ALA	2.3
3	V	184	ALA	2.3
2	W	217	ARG	2.3
3	V	172	THR	2.3
3	Z	147	GLN	2.3
3	Z	162	SER	2.3
1	B	208	MET	2.3
1	F	206	PRO	2.3
1	C	248	HIS	2.2
2	J	134	SER	2.2
3	X	77	SER	2.2
3	Z	107	LYS	2.2
3	N	195	GLU	2.2
3	Z	195	GLU	2.2
3	V	139	PHE	2.2
3	Z	102	THR	2.2
1	F	208	MET	2.2
2	I	164	GLY	2.2
2	Y	213	LYS	2.2
3	M	106	ILE	2.2
3	V	133	VAL	2.2
1	E	248	HIS	2.2
3	Z	164	THR	2.2
2	Y	115	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	247	SER	2.2
3	Z	121	SER	2.2
1	B	259	ASP	2.2
3	Z	185	ASP	2.2
3	Z	148	TRP	2.2
3	M	81	PRO	2.2
3	M	204	PRO	2.2
3	V	115	VAL	2.2
3	V	178	THR	2.2
3	V	186	TYR	2.2
1	D	217	SER	2.2
2	W	134	SER	2.2
2	Y	222	SER	2.2
3	V	168	SER	2.2
1	C	233	ARG	2.2
3	N	81	PRO	2.2
3	N	106	ILE	2.1
3	Z	71	ASP	2.1
3	V	81	PRO	2.1
3	Z	72	PHE	2.1
1	D	290	HIS	2.1
2	Y	95	TYR	2.1
3	V	177	SER	2.1
3	Z	182	SER	2.1
3	Z	141	PRO	2.1
3	V	189	HIS	2.1
3	N	196	VAL	2.1
1	B	204	THR	2.1
1	D	262	GLY	2.1
3	M	206	THR	2.1
3	V	200	GLY	2.1
3	V	212	GLY	2.1
3	M	114	SER	2.1
3	N	194	CYS	2.1
3	Z	66	SER	2.1
3	L	41	PRO	2.1
3	M	84	PHE	2.1
3	M	209	PHE	2.1
2	I	142	THR	2.1
1	D	259	ASP	2.1
3	V	151	ASP	2.1
1	D	232	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	M	194	CYS	2.1
3	M	147	GLN	2.0
2	I	144	ALA	2.0
3	V	112	ALA	2.0
3	X	187	GLU	2.0
1	C	212	THR	2.0
1	C	253	TRP	2.0
2	Y	216	LYS	2.0
3	V	109	THR	2.0
1	D	255	ASP	2.0
2	Y	8	SER	2.0
1	E	290	HIS	2.0
3	V	160	GLN	2.0
3	M	78	ARG	2.0
2	Y	125	GLY	2.0
3	M	200	GLY	2.0
2	I	198	THR	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
4	NAG	F	401	14/15	0.66	0.17	89,96,101,101	0
5	EDO	U	301	4/4	0.78	0.27	42,42,45,53	0
4	NAG	F	402	14/15	0.84	0.15	59,63,69,73	0
4	NAG	E	401	14/15	0.84	0.15	57,60,65,65	0
5	EDO	L	301	4/4	0.88	0.14	46,47,49,51	0
4	NAG	B	401	14/15	0.88	0.10	31,39,42,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	E	402	4/4	0.89	0.21	32,33,34,34	0
5	EDO	B	402	4/4	0.91	0.20	28,29,31,31	0
4	NAG	A	401	14/15	0.92	0.09	35,38,45,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.