



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:57 PM UTC

PDB ID : 8RT1 / pdb\_00008rt1  
Title : BTV15 VP5 at pH 9.0  
Authors : Sutton, G.C.; Stuart, D.I.  
Deposited on : 2024-01-25  
Resolution : 2.80 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

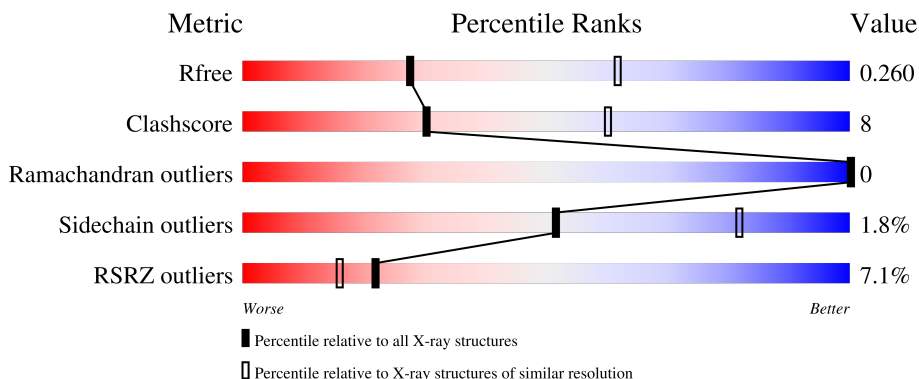
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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.



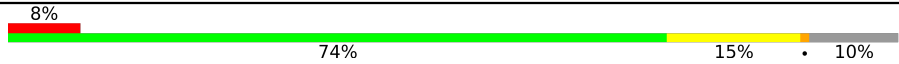
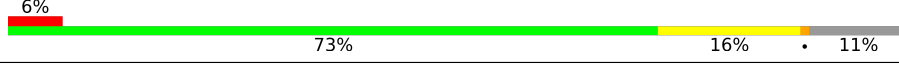
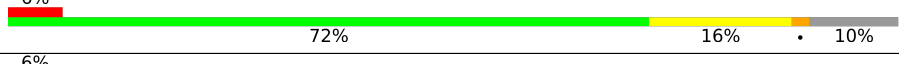

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	490	 6% 75% 16% • 8%
1	B	490	 7% 73% 15% • 10%
1	C	490	 6% 71% 18% • 10%
1	D	490	 4% 73% 14% • 12%
1	E	490	 7% 72% 16% • 10%

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Mol	Chain	Length	Quality of chain
1	F	490	 8% 74% 15% 10%
1	G	490	 6% 73% 16% 11%
1	H	490	 6% 72% 16% 10%
1	I	490	 6% 72% 15% 12%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 31370 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 Outer capsid protein VP5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	451	Total 3585	C 2254	N 636	O 682	Se 13	0	0	0
1	B	440	Total 3485	C 2193	N 612	O 668	Se 12	0	0	0
1	C	439	Total 3479	C 2190	N 611	O 666	Se 12	0	0	0
1	D	432	Total 3431	C 2160	N 603	O 655	Se 13	0	0	0
1	E	442	Total 3516	C 2212	N 623	O 668	Se 13	0	0	0
1	F	439	Total 3479	C 2190	N 611	O 666	Se 12	0	0	0
1	G	438	Total 3471	C 2186	N 609	O 664	Se 12	0	0	0
1	H	440	Total 3484	C 2193	N 612	O 667	Se 12	0	0	0
1	I	433	Total 3440	C 2164	N 607	O 657	Se 12	0	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	HIS	-	expression tag	UNP R4J9Y2
A	39	HIS	-	expression tag	UNP R4J9Y2
A	40	HIS	-	expression tag	UNP R4J9Y2
A	41	HIS	-	expression tag	UNP R4J9Y2
A	42	HIS	-	expression tag	UNP R4J9Y2
A	43	HIS	-	expression tag	UNP R4J9Y2
A	178	ALA	VAL	conflict	UNP R4J9Y2
B	38	HIS	-	expression tag	UNP R4J9Y2
B	39	HIS	-	expression tag	UNP R4J9Y2
B	40	HIS	-	expression tag	UNP R4J9Y2
B	41	HIS	-	expression tag	UNP R4J9Y2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	42	HIS	-	expression tag	UNP R4J9Y2
B	43	HIS	-	expression tag	UNP R4J9Y2
B	178	ALA	VAL	conflict	UNP R4J9Y2
C	38	HIS	-	expression tag	UNP R4J9Y2
C	39	HIS	-	expression tag	UNP R4J9Y2
C	40	HIS	-	expression tag	UNP R4J9Y2
C	41	HIS	-	expression tag	UNP R4J9Y2
C	42	HIS	-	expression tag	UNP R4J9Y2
C	43	HIS	-	expression tag	UNP R4J9Y2
C	178	ALA	VAL	conflict	UNP R4J9Y2
D	38	HIS	-	expression tag	UNP R4J9Y2
D	39	HIS	-	expression tag	UNP R4J9Y2
D	40	HIS	-	expression tag	UNP R4J9Y2
D	41	HIS	-	expression tag	UNP R4J9Y2
D	42	HIS	-	expression tag	UNP R4J9Y2
D	43	HIS	-	expression tag	UNP R4J9Y2
D	178	ALA	VAL	conflict	UNP R4J9Y2
E	38	HIS	-	expression tag	UNP R4J9Y2
E	39	HIS	-	expression tag	UNP R4J9Y2
E	40	HIS	-	expression tag	UNP R4J9Y2
E	41	HIS	-	expression tag	UNP R4J9Y2
E	42	HIS	-	expression tag	UNP R4J9Y2
E	43	HIS	-	expression tag	UNP R4J9Y2
E	178	ALA	VAL	conflict	UNP R4J9Y2
F	38	HIS	-	expression tag	UNP R4J9Y2
F	39	HIS	-	expression tag	UNP R4J9Y2
F	40	HIS	-	expression tag	UNP R4J9Y2
F	41	HIS	-	expression tag	UNP R4J9Y2
F	42	HIS	-	expression tag	UNP R4J9Y2
F	43	HIS	-	expression tag	UNP R4J9Y2
F	178	ALA	VAL	conflict	UNP R4J9Y2
G	38	HIS	-	expression tag	UNP R4J9Y2
G	39	HIS	-	expression tag	UNP R4J9Y2
G	40	HIS	-	expression tag	UNP R4J9Y2
G	41	HIS	-	expression tag	UNP R4J9Y2
G	42	HIS	-	expression tag	UNP R4J9Y2
G	43	HIS	-	expression tag	UNP R4J9Y2
G	178	ALA	VAL	conflict	UNP R4J9Y2
H	38	HIS	-	expression tag	UNP R4J9Y2
H	39	HIS	-	expression tag	UNP R4J9Y2
H	40	HIS	-	expression tag	UNP R4J9Y2
H	41	HIS	-	expression tag	UNP R4J9Y2

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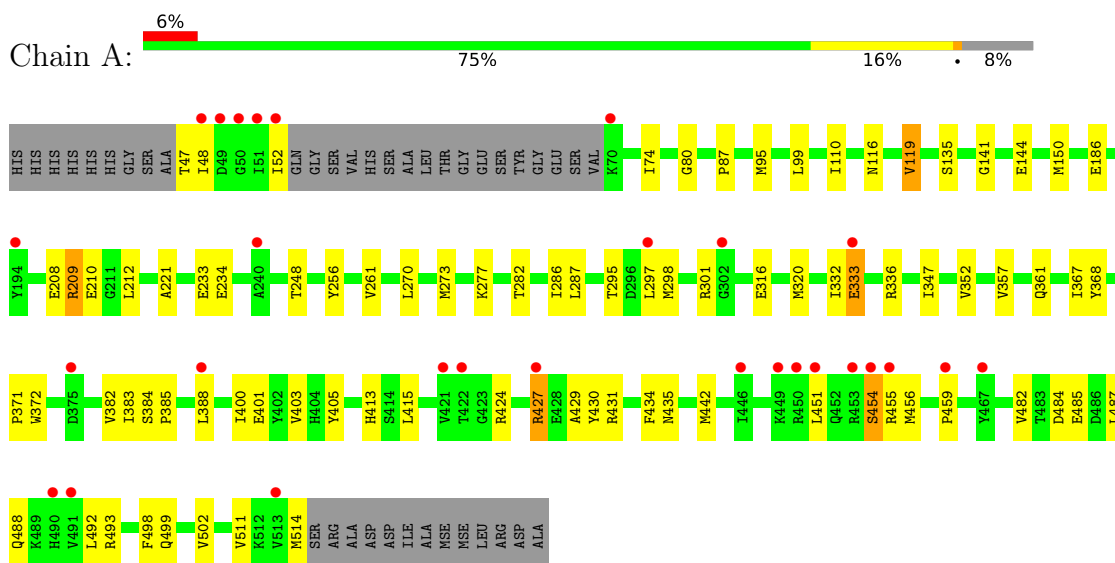
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Chain	Residue	Modelled	Actual	Comment	Reference
H	42	HIS	-	expression tag	UNP R4J9Y2
H	43	HIS	-	expression tag	UNP R4J9Y2
H	178	ALA	VAL	conflict	UNP R4J9Y2
I	38	HIS	-	expression tag	UNP R4J9Y2
I	39	HIS	-	expression tag	UNP R4J9Y2
I	40	HIS	-	expression tag	UNP R4J9Y2
I	41	HIS	-	expression tag	UNP R4J9Y2
I	42	HIS	-	expression tag	UNP R4J9Y2
I	43	HIS	-	expression tag	UNP R4J9Y2
I	178	ALA	VAL	conflict	UNP R4J9Y2

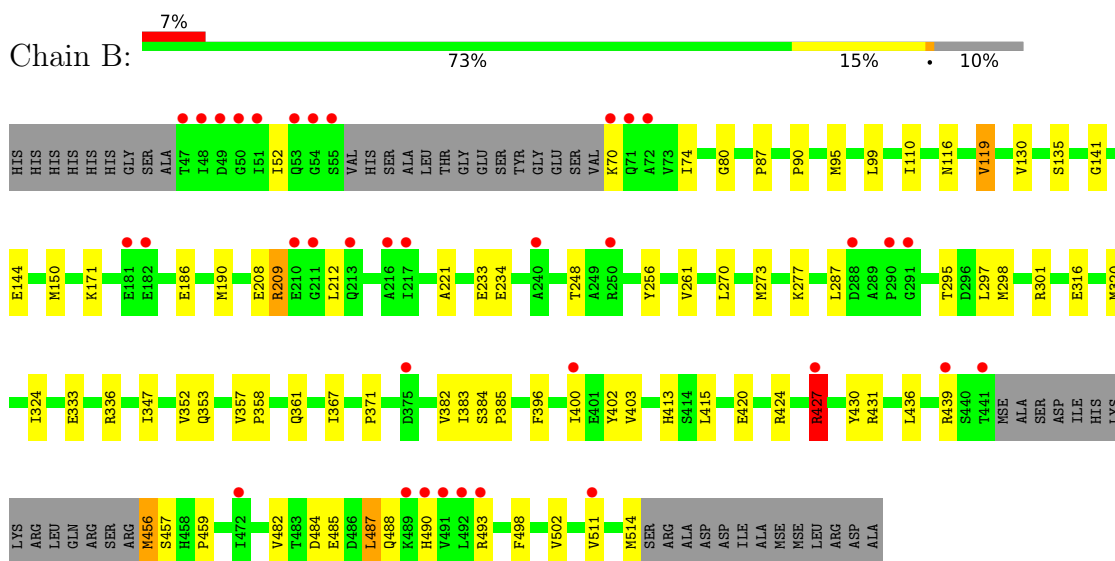
### 3 Residue-property plots [i](#)

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.

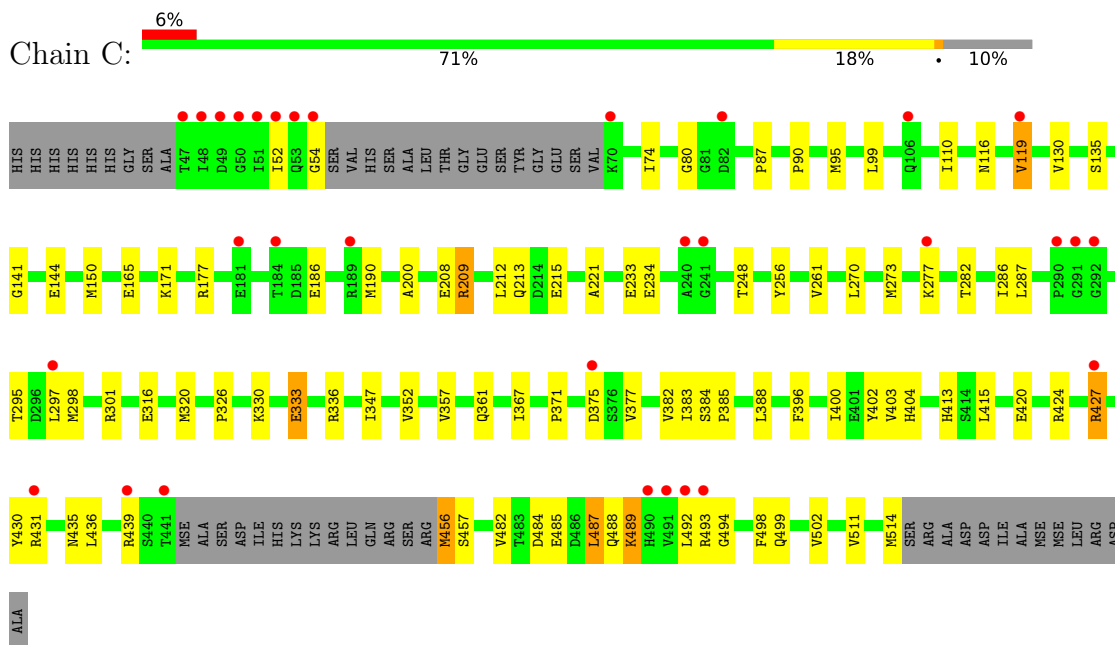
- Molecule 1: Outer capsid protein VP5



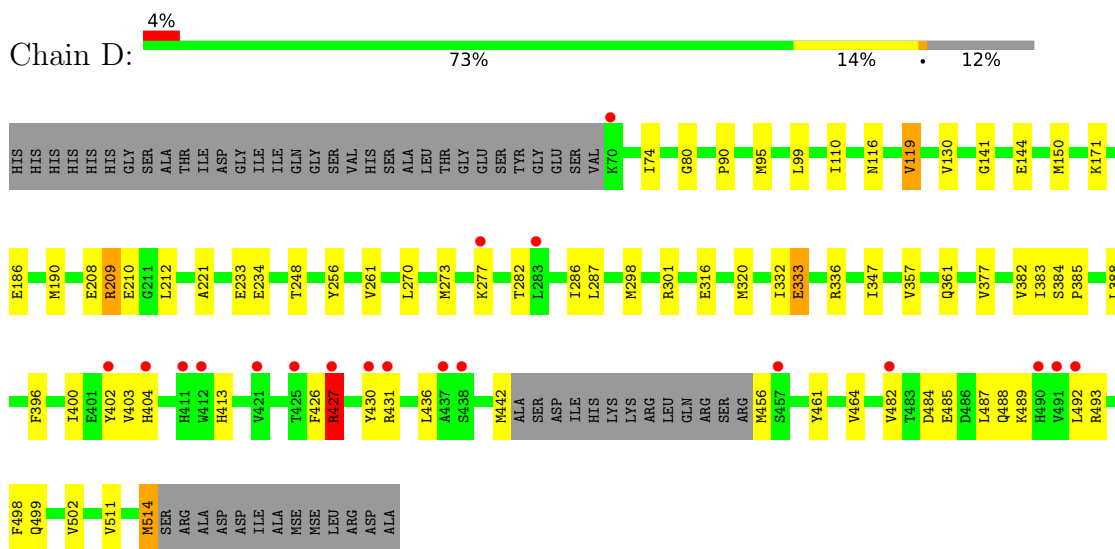
- Molecule 1: Outer capsid protein VP5



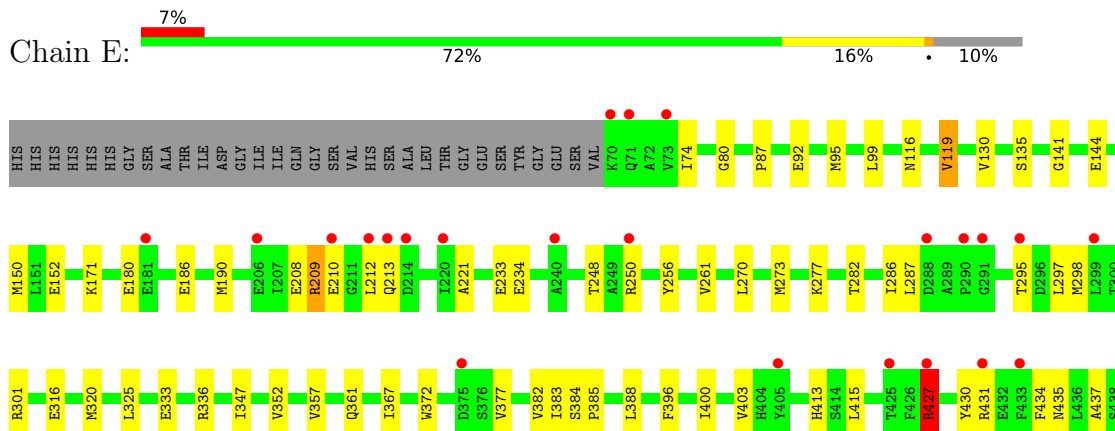
- Molecule 1: Outer capsid protein VP5

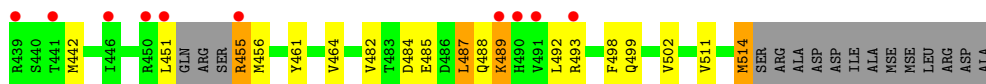


- Molecule 1: Outer capsid protein VP5

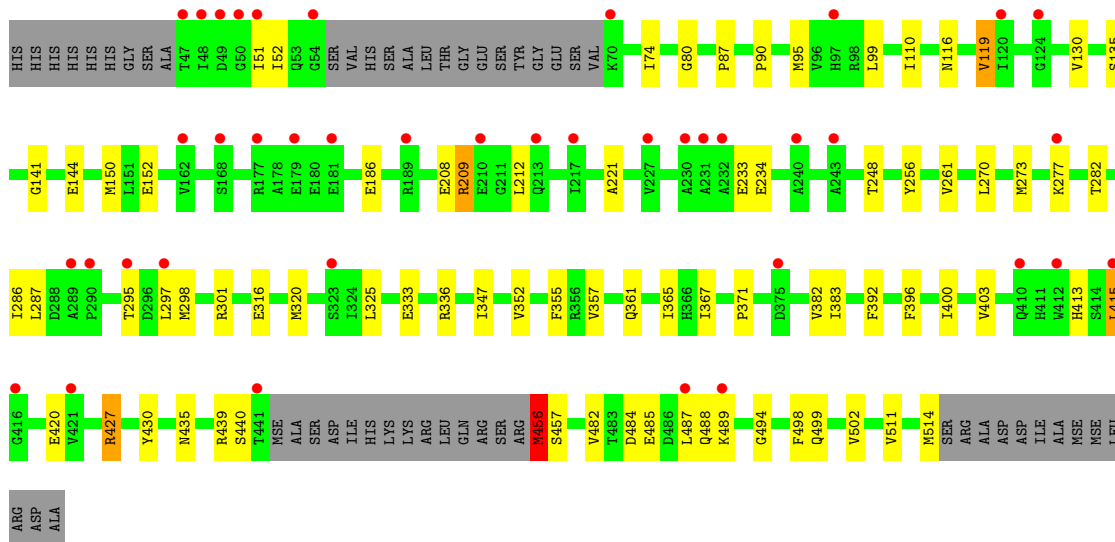
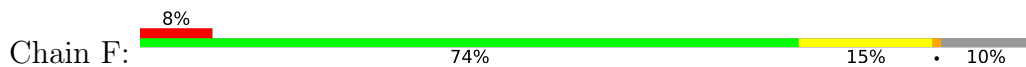


- Molecule 1: Outer capsid protein VP5

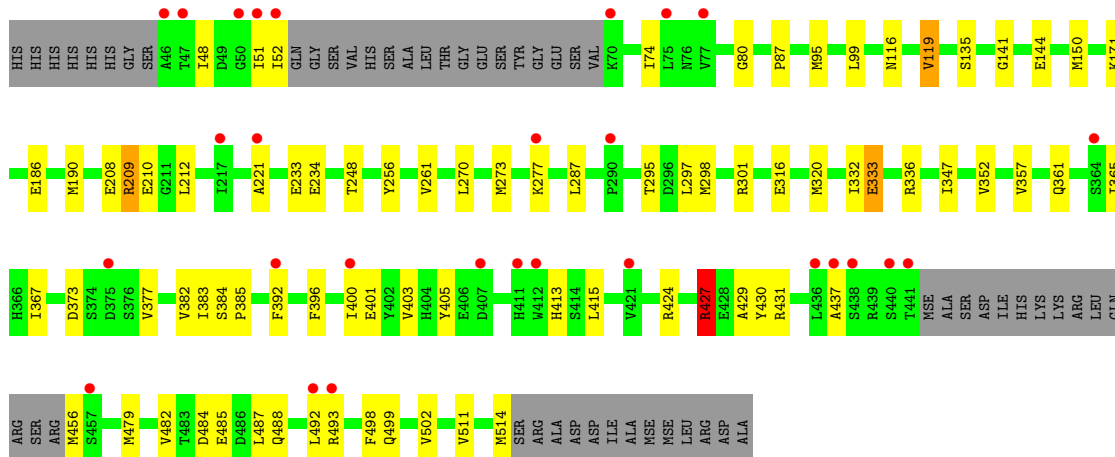
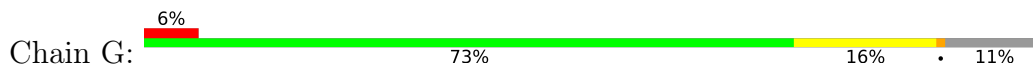




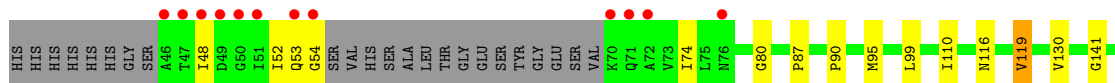
- Molecule 1: Outer capsid protein VP5

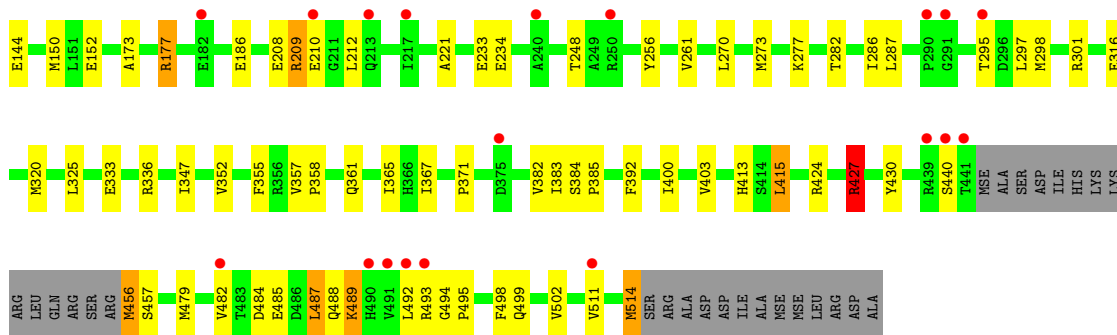


- Molecule 1: Outer capsid protein VP5

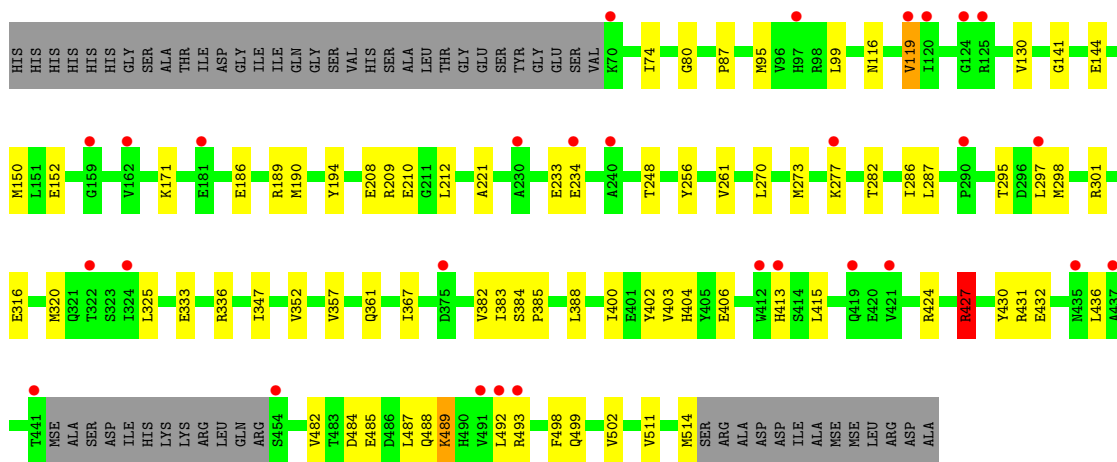


- Molecule 1: Outer capsid protein VP5





• Molecule 1: Outer capsid protein VP5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.40Å 142.21Å 142.15Å 119.54° 96.09° 95.80°	Depositor
Resolution (Å)	46.63 – 2.80 46.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (46.63-2.80) 98.3 (46.63-2.80)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.240 , 0.261 0.239 , 0.260	Depositor DCC
$R_{free}$ test set	7251 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.5	Xtrriage
Anisotropy	0.029	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.009 for -h,-l,-k	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31370	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.40% 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

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	0.96	2/3634 (0.1%)	1.50	2/4878 (0.0%)
1	B	0.95	1/3534 (0.0%)	1.49	6/4749 (0.1%)
1	C	0.96	1/3528 (0.0%)	1.49	10/4741 (0.2%)
1	D	0.96	2/3480 (0.1%)	1.49	7/4675 (0.1%)
1	E	0.96	3/3565 (0.1%)	1.49	5/4785 (0.1%)
1	F	0.96	2/3528 (0.1%)	1.49	6/4741 (0.1%)
1	G	0.96	2/3520 (0.1%)	1.48	3/4731 (0.1%)
1	H	0.96	1/3533 (0.0%)	1.49	6/4748 (0.1%)
1	I	0.95	0/3489	1.49	6/4687 (0.1%)
All	All	0.96	14/31811 (0.0%)	1.49	51/42735 (0.1%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	1	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	1	8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	456	MSE	SE-CE	7.29	2.17	1.95
1	E	442	MSE	SE-CE	6.07	2.13	1.95
1	A	454	SER	CA-CB	-5.98	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	456	MSE	SE-CE	5.73	2.12	1.95
1	H	456	MSE	CG-SE	5.58	2.12	1.95
1	A	456	MSE	SE-CE	5.52	2.12	1.95
1	D	442	MSE	SE-CE	5.46	2.11	1.95
1	G	456	MSE	CG-SE	5.40	2.11	1.95
1	F	456	MSE	CG-SE	5.39	2.11	1.95
1	E	456	MSE	SE-CE	5.33	2.11	1.95
1	B	456	MSE	SE-CE	5.25	2.11	1.95
1	F	456	MSE	SE-CE	5.10	2.10	1.95
1	D	456	MSE	SE-CE	5.03	2.10	1.95
1	E	442	MSE	CG-SE	5.00	2.10	1.95

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	427	ARG	NE-CZ-NH2	6.74	125.26	119.20
1	C	177	ARG	NE-CZ-NH2	6.39	124.95	119.20
1	F	489	LYS	CB-CG-CD	5.79	124.62	111.30
1	D	489	LYS	CB-CG-CD	5.62	124.22	111.30
1	G	119	VAL	N-CA-CB	5.62	118.18	110.54
1	E	119	VAL	N-CA-CB	5.56	118.11	110.54
1	C	119	VAL	N-CA-CB	5.54	118.07	110.54
1	B	119	VAL	N-CA-CB	5.53	118.06	110.54
1	I	119	VAL	N-CA-CB	5.52	118.04	110.54
1	I	489	LYS	CB-CA-C	5.51	119.32	109.29
1	H	119	VAL	N-CA-CB	5.51	118.03	110.54
1	H	489	LYS	CB-CG-CD	5.49	123.92	111.30
1	H	427	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	F	119	VAL	N-CA-CB	5.42	117.91	110.54
1	D	119	VAL	N-CA-CB	5.42	117.91	110.54
1	E	427	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	A	119	VAL	N-CA-CB	5.36	117.83	110.54
1	I	427	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	C	489	LYS	CB-CG-CD	5.27	123.43	111.30
1	F	90	PRO	CA-C-N	5.27	125.79	119.94
1	F	90	PRO	C-N-CA	5.27	125.79	119.94
1	D	427	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	E	489	LYS	CB-CA-C	5.25	118.84	109.29
1	I	432	GLU	CA-C-O	-5.23	115.33	120.82
1	I	404	HIS	CB-CA-C	-5.20	100.72	109.72
1	B	439	ARG	CG-CD-NE	5.20	123.43	112.00
1	E	455	ARG	CG-CD-NE	-5.19	100.57	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	GLU	CB-CA-C	5.19	118.30	109.53
1	I	210	GLU	CB-CA-C	5.18	120.27	109.95
1	B	427	ARG	CG-CD-NE	-5.18	100.60	112.00
1	D	404	HIS	CB-CA-C	-5.17	100.77	109.72
1	C	420	GLU	CB-CA-C	5.15	118.23	109.53
1	G	427	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	D	210	GLU	CB-CA-C	5.13	120.15	109.95
1	H	90	PRO	CA-C-N	5.09	125.59	119.94
1	H	90	PRO	C-N-CA	5.09	125.59	119.94
1	H	210	GLU	CB-CA-C	5.06	120.03	109.95
1	D	90	PRO	CA-C-N	5.06	125.56	119.94
1	D	90	PRO	C-N-CA	5.06	125.56	119.94
1	C	165	GLU	CA-C-N	5.05	125.55	119.94
1	C	165	GLU	C-N-CA	5.05	125.55	119.94
1	C	375	ASP	CB-CA-C	5.05	118.53	110.09
1	G	210	GLU	CB-CA-C	5.04	119.98	109.95
1	C	90	PRO	CA-C-N	5.04	125.53	119.94
1	C	90	PRO	C-N-CA	5.04	125.53	119.94
1	C	404	HIS	CB-CA-C	-5.03	101.02	109.72
1	E	210	GLU	CB-CA-C	5.02	119.94	109.95
1	A	210	GLU	CB-CA-C	5.01	119.93	109.95
1	F	420	GLU	CB-CA-C	5.01	118.01	109.84
1	B	90	PRO	CA-C-N	5.01	125.50	119.94
1	B	90	PRO	C-N-CA	5.01	125.50	119.94

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	456	MSE	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	ARG	Sidechain
1	B	427	ARG	Sidechain
1	C	427	ARG	Sidechain
1	D	427	ARG	Sidechain
1	E	427	ARG	Sidechain
1	G	427	ARG	Sidechain
1	H	427	ARG	Sidechain
1	I	427	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3589	66	0
1	B	3485	0	3475	67	0
1	C	3479	0	3470	63	0
1	D	3431	0	3422	50	0
1	E	3516	0	3517	61	0
1	F	3479	0	3470	68	0
1	G	3471	0	3464	62	0
1	H	3484	0	3475	64	0
1	I	3440	0	3431	53	0
All	All	31370	0	31313	524	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 8.

All (524) 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)
1:B:431:ARG:CG	1:B:456:MSE:HE1	1.37	1.51
1:F:427:ARG:NH1	1:F:456:MSE:HE1	1.18	1.45
1:C:456:MSE:SE	1:C:456:MSE:CE	2.17	1.43
1:B:431:ARG:CD	1:B:456:MSE:HE1	1.54	1.37
1:D:402:TYR:CZ	1:D:436:LEU:HD23	1.68	1.28
1:A:401:GLU:OE1	1:A:442:MSE:HE1	1.40	1.22
1:F:427:ARG:NH1	1:F:456:MSE:CE	2.10	1.14
1:B:431:ARG:CD	1:B:456:MSE:CE	2.25	1.14
1:B:431:ARG:HG2	1:B:456:MSE:CE	1.78	1.13
1:F:427:ARG:HH12	1:F:456:MSE:CE	1.61	1.09
1:B:431:ARG:CG	1:B:456:MSE:CE	2.33	1.04
1:D:402:TYR:CE1	1:D:436:LEU:HD23	1.91	1.04
1:C:52:ILE:HA	1:C:488:GLN:OE1	1.60	1.01
1:I:402:TYR:CZ	1:I:436:LEU:HD22	1.96	1.00
1:B:431:ARG:HG2	1:B:456:MSE:HE1	1.03	0.99
1:G:150:MSE:HE2	1:G:261:VAL:HG11	1.46	0.97
1:E:150:MSE:HE2	1:E:261:VAL:HG11	1.47	0.97
1:H:52:ILE:HA	1:H:488:GLN:OE1	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:150:MSE:HE2	1:H:261:VAL:HG11	1.48	0.96
1:A:150:MSE:HE2	1:A:261:VAL:HG11	1.47	0.95
1:D:402:TYR:OH	1:D:436:LEU:HD23	1.64	0.95
1:B:150:MSE:HE2	1:B:261:VAL:HG11	1.49	0.95
1:I:150:MSE:HE2	1:I:261:VAL:HG11	1.48	0.95
1:F:150:MSE:HE2	1:F:261:VAL:HG11	1.48	0.94
1:D:150:MSE:HE2	1:D:261:VAL:HG11	1.47	0.93
1:C:150:MSE:HE2	1:C:261:VAL:HG11	1.48	0.93
1:D:150:MSE:CE	1:D:261:VAL:HG11	2.00	0.91
1:C:54:GLY:HA3	1:C:489:LYS:HG3	1.52	0.91
1:F:150:MSE:CE	1:F:261:VAL:HG11	2.01	0.90
1:E:150:MSE:CE	1:E:261:VAL:HG11	2.00	0.90
1:A:150:MSE:CE	1:A:261:VAL:HG11	2.01	0.90
1:B:150:MSE:CE	1:B:261:VAL:HG11	2.01	0.90
1:G:150:MSE:CE	1:G:261:VAL:HG11	2.00	0.90
1:I:150:MSE:CE	1:I:261:VAL:HG11	2.02	0.89
1:C:52:ILE:HG23	1:C:488:GLN:HB3	1.53	0.89
1:C:150:MSE:CE	1:C:261:VAL:HG11	2.02	0.89
1:H:150:MSE:CE	1:H:261:VAL:HG11	2.02	0.88
1:B:270:LEU:HD22	1:B:273:MSE:HE3	1.56	0.87
1:E:270:LEU:HD22	1:E:273:MSE:HE3	1.56	0.87
1:A:270:LEU:HD22	1:A:273:MSE:HE3	1.55	0.87
1:D:270:LEU:HD22	1:D:273:MSE:HE3	1.56	0.86
1:G:270:LEU:HD22	1:G:273:MSE:HE3	1.56	0.86
1:H:270:LEU:HD22	1:H:273:MSE:HE3	1.57	0.86
1:F:400:ILE:HD11	1:F:440:SER:HB3	1.57	0.86
1:C:270:LEU:HD22	1:C:273:MSE:HE3	1.59	0.85
1:I:270:LEU:HD22	1:I:273:MSE:HE3	1.56	0.85
1:F:270:LEU:HD22	1:F:273:MSE:HE3	1.58	0.85
1:H:400:ILE:HD11	1:H:440:SER:HB3	1.60	0.84
1:B:431:ARG:HD3	1:B:456:MSE:CE	2.07	0.84
1:A:273:MSE:HE2	1:A:316:GLU:HB3	1.61	0.83
1:B:402:TYR:CD2	1:B:436:LEU:HD23	2.13	0.83
1:I:402:TYR:CE1	1:I:436:LEU:HD22	2.13	0.83
1:F:273:MSE:HE2	1:F:316:GLU:HB3	1.62	0.82
1:H:52:ILE:HG23	1:H:488:GLN:HB3	1.59	0.82
1:A:52:ILE:HG23	1:A:488:GLN:HB3	1.62	0.82
1:A:435:ASN:HB2	1:A:455:ARG:HH11	1.44	0.81
1:B:357:VAL:HG23	1:B:415:LEU:HD12	1.62	0.81
1:I:273:MSE:HE2	1:I:316:GLU:HB3	1.63	0.81
1:B:431:ARG:HD2	1:B:456:MSE:SE	2.30	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:MSE:HE2	1:D:316:GLU:HB3	1.62	0.81
1:G:273:MSE:HE2	1:G:316:GLU:HB3	1.63	0.81
1:F:427:ARG:HH11	1:F:456:MSE:HE1	1.44	0.80
1:D:402:TYR:OH	1:D:436:LEU:CD2	2.30	0.79
1:A:401:GLU:OE1	1:A:442:MSE:CE	2.27	0.79
1:H:273:MSE:HE2	1:H:316:GLU:HB3	1.64	0.79
1:B:273:MSE:HE2	1:B:316:GLU:HB3	1.64	0.78
1:E:273:MSE:HE2	1:E:316:GLU:HB3	1.63	0.78
1:B:431:ARG:HD3	1:B:456:MSE:HE1	1.65	0.78
1:B:431:ARG:HD2	1:B:456:MSE:CE	2.11	0.78
1:C:273:MSE:HE2	1:C:316:GLU:HB3	1.64	0.77
1:F:382:VAL:HG21	1:F:392:PHE:CZ	2.20	0.76
1:H:382:VAL:HG21	1:H:392:PHE:CZ	2.20	0.76
1:G:382:VAL:HG21	1:G:392:PHE:CZ	2.20	0.75
1:D:402:TYR:CE1	1:D:436:LEU:CD2	2.70	0.74
1:B:295:THR:HG22	1:B:297:LEU:H	1.55	0.72
1:G:48:ILE:HD13	1:G:479:MSE:HE1	1.71	0.72
1:C:295:THR:HG22	1:C:297:LEU:H	1.55	0.72
1:G:382:VAL:HG21	1:G:392:PHE:CE2	2.25	0.72
1:H:295:THR:HG22	1:H:297:LEU:H	1.55	0.72
1:H:54:GLY:HA3	1:H:489:LYS:HG3	1.70	0.71
1:F:295:THR:HG22	1:F:297:LEU:H	1.55	0.71
1:G:295:THR:HG22	1:G:297:LEU:H	1.55	0.71
1:A:295:THR:HG22	1:A:297:LEU:H	1.55	0.70
1:I:295:THR:HG22	1:I:297:LEU:H	1.55	0.70
1:F:427:ARG:HH12	1:F:456:MSE:HE1	0.89	0.69
1:F:52:ILE:HA	1:F:488:GLN:OE1	1.93	0.69
1:E:295:THR:HG22	1:E:297:LEU:H	1.55	0.68
1:H:382:VAL:HG21	1:H:392:PHE:CE2	2.28	0.68
1:E:400:ILE:O	1:E:400:ILE:HG22	1.95	0.67
1:F:355:PHE:O	1:F:415:LEU:HD11	1.95	0.67
1:G:51:ILE:HG23	1:G:401:GLU:O	1.94	0.67
1:F:382:VAL:HG21	1:F:392:PHE:CE2	2.29	0.67
1:C:431:ARG:HD2	1:C:456:MSE:HE1	1.76	0.66
1:F:400:ILE:HG22	1:F:400:ILE:O	1.94	0.66
1:A:371:PRO:HG2	1:A:454:SER:HA	1.78	0.66
1:H:400:ILE:HG22	1:H:400:ILE:O	1.94	0.66
1:B:52:ILE:HA	1:B:488:GLN:OE1	1.94	0.66
1:D:400:ILE:HG22	1:D:400:ILE:O	1.95	0.65
1:C:431:ARG:HD2	1:C:456:MSE:CE	2.26	0.65
1:I:400:ILE:HG22	1:I:400:ILE:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:400:ILE:O	1:G:400:ILE:HG22	1.96	0.65
1:A:400:ILE:HG22	1:A:400:ILE:O	1.94	0.64
1:G:48:ILE:HG22	1:G:482:VAL:CG2	2.27	0.64
1:B:400:ILE:O	1:B:400:ILE:HG22	1.95	0.64
1:F:357:VAL:HG23	1:F:415:LEU:HD13	1.81	0.63
1:C:400:ILE:HG22	1:C:400:ILE:O	1.96	0.63
1:H:355:PHE:O	1:H:415:LEU:HD11	1.98	0.62
1:I:233:GLU:HG2	1:I:248:THR:HG22	1.81	0.62
1:G:52:ILE:HA	1:G:488:GLN:OE1	2.00	0.62
1:F:233:GLU:HG2	1:F:248:THR:HG22	1.81	0.62
1:C:215:GLU:CD	1:C:493:ARG:HH12	2.07	0.62
1:G:233:GLU:HG2	1:G:248:THR:HG22	1.82	0.62
1:A:372:TRP:CH2	1:A:451:LEU:HD23	2.35	0.62
1:H:53:GLN:OE1	1:H:485:GLU:HB2	2.00	0.62
1:C:233:GLU:HG2	1:C:248:THR:HG22	1.82	0.61
1:G:382:VAL:CG2	1:G:392:PHE:CE2	2.84	0.61
1:E:233:GLU:HG2	1:E:248:THR:HG22	1.83	0.61
1:E:435:ASN:HB2	1:E:455:ARG:HH11	1.64	0.61
1:E:295:THR:HG22	1:E:297:LEU:N	2.17	0.60
1:B:233:GLU:HG2	1:B:248:THR:HG22	1.84	0.60
1:F:295:THR:HG22	1:F:297:LEU:N	2.17	0.60
1:I:295:THR:HG22	1:I:297:LEU:N	2.16	0.60
1:A:295:THR:HG22	1:A:297:LEU:N	2.16	0.60
1:F:357:VAL:HG23	1:F:415:LEU:CD1	2.31	0.60
1:H:295:THR:HG22	1:H:297:LEU:N	2.17	0.60
1:D:233:GLU:HG2	1:D:248:THR:HG22	1.84	0.60
1:B:295:THR:HG22	1:B:297:LEU:N	2.17	0.59
1:A:434:PHE:HD2	1:A:455:ARG:HA	1.68	0.59
1:E:372:TRP:CH2	1:E:451:LEU:HD23	2.37	0.59
1:H:233:GLU:HG2	1:H:248:THR:HG22	1.84	0.59
1:A:233:GLU:HG2	1:A:248:THR:HG22	1.84	0.59
1:B:402:TYR:CE2	1:B:436:LEU:HD23	2.38	0.59
1:G:295:THR:HG22	1:G:297:LEU:N	2.16	0.59
1:C:295:THR:HG22	1:C:297:LEU:N	2.16	0.59
1:F:209:ARG:HA	1:F:212:LEU:HD13	1.85	0.59
1:B:298:MSE:HG2	1:B:301:ARG:HH21	1.69	0.58
1:A:435:ASN:HB2	1:A:455:ARG:NH1	2.15	0.58
1:C:402:TYR:CE2	1:C:436:LEU:HD23	2.38	0.58
1:F:52:ILE:HD11	1:F:403:VAL:HB	1.86	0.58
1:H:208:GLU:HG2	1:H:221:ALA:HA	1.86	0.58
1:H:382:VAL:CG2	1:H:392:PHE:CE2	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:TRP:CZ2	1:E:451:LEU:HD23	2.39	0.57
1:A:52:ILE:HA	1:A:488:GLN:OE1	2.04	0.57
1:A:434:PHE:CD2	1:A:455:ARG:HA	2.39	0.57
1:H:357:VAL:HG23	1:H:415:LEU:CD1	2.35	0.57
1:C:208:GLU:HG2	1:C:221:ALA:HA	1.86	0.57
1:F:382:VAL:CG2	1:F:392:PHE:CE2	2.88	0.57
1:B:209:ARG:HA	1:B:212:LEU:HD13	1.87	0.57
1:F:208:GLU:HG2	1:F:221:ALA:HA	1.85	0.57
1:G:48:ILE:HG22	1:G:482:VAL:HG22	1.86	0.56
1:B:402:TYR:CD2	1:B:436:LEU:CD2	2.88	0.56
1:E:208:GLU:HG2	1:E:221:ALA:HA	1.88	0.56
1:E:361:GLN:HA	1:E:383:ILE:CD1	2.36	0.56
1:G:361:GLN:HA	1:G:383:ILE:CD1	2.35	0.56
1:H:209:ARG:HA	1:H:212:LEU:HD13	1.87	0.56
1:I:208:GLU:HG2	1:I:221:ALA:HA	1.86	0.56
1:F:361:GLN:HA	1:F:383:ILE:CD1	2.35	0.56
1:I:361:GLN:HA	1:I:383:ILE:CD1	2.36	0.56
1:B:208:GLU:HG2	1:B:221:ALA:HA	1.87	0.56
1:C:209:ARG:HA	1:C:212:LEU:HD13	1.86	0.56
1:C:361:GLN:HA	1:C:383:ILE:CD1	2.36	0.56
1:D:361:GLN:HA	1:D:383:ILE:CD1	2.36	0.56
1:A:361:GLN:HA	1:A:383:ILE:CD1	2.36	0.56
1:B:427:ARG:HA	1:B:430:TYR:CE2	2.41	0.56
1:H:357:VAL:HG23	1:H:415:LEU:HD13	1.87	0.56
1:B:361:GLN:HA	1:B:383:ILE:CD1	2.35	0.56
1:A:427:ARG:HA	1:A:430:TYR:CE2	2.41	0.56
1:G:333:GLU:OE1	1:G:336:ARG:NH1	2.39	0.56
1:H:361:GLN:HA	1:H:383:ILE:CD1	2.36	0.56
1:A:333:GLU:OE1	1:A:336:ARG:NH1	2.39	0.55
1:A:209:ARG:HA	1:A:212:LEU:HD13	1.88	0.55
1:C:333:GLU:OE1	1:C:336:ARG:NH1	2.40	0.55
1:D:333:GLU:OE1	1:D:336:ARG:NH1	2.40	0.55
1:G:209:ARG:HA	1:G:212:LEU:HD13	1.88	0.55
1:B:333:GLU:OE1	1:B:336:ARG:NH1	2.40	0.55
1:E:333:GLU:OE1	1:E:336:ARG:NH1	2.40	0.55
1:G:208:GLU:HG2	1:G:221:ALA:HA	1.88	0.55
1:H:427:ARG:HA	1:H:430:TYR:CE2	2.41	0.55
1:A:400:ILE:O	1:A:400:ILE:CG2	2.55	0.55
1:B:431:ARG:HD3	1:B:456:MSE:HE2	1.86	0.55
1:C:427:ARG:HA	1:C:430:TYR:CE2	2.42	0.55
1:D:209:ARG:HA	1:D:212:LEU:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:MSE:HG2	1:G:301:ARG:HH21	1.72	0.55
1:I:209:ARG:HA	1:I:212:LEU:HD13	1.89	0.55
1:E:209:ARG:HA	1:E:212:LEU:HD13	1.88	0.55
1:F:427:ARG:HA	1:F:430:TYR:CE2	2.42	0.55
1:I:333:GLU:OE1	1:I:336:ARG:NH1	2.39	0.55
1:I:427:ARG:HA	1:I:430:TYR:CE2	2.42	0.55
1:E:427:ARG:HA	1:E:430:TYR:CE2	2.42	0.55
1:F:333:GLU:OE1	1:F:336:ARG:NH1	2.39	0.55
1:H:333:GLU:OE1	1:H:336:ARG:NH1	2.40	0.54
1:A:47:THR:HG22	1:A:47:THR:O	2.07	0.54
1:D:427:ARG:HA	1:D:430:TYR:CE2	2.42	0.54
1:E:400:ILE:O	1:E:400:ILE:CG2	2.56	0.54
1:G:427:ARG:HA	1:G:430:TYR:CE2	2.43	0.54
1:B:400:ILE:O	1:B:400:ILE:CG2	2.55	0.54
1:E:95:MSE:HG2	1:F:99:LEU:HD11	1.90	0.54
1:G:382:VAL:CG2	1:G:392:PHE:CZ	2.90	0.54
1:G:52:ILE:HD11	1:G:396:PHE:CE2	2.42	0.54
1:A:208:GLU:HG2	1:A:221:ALA:HA	1.89	0.54
1:A:372:TRP:CZ2	1:A:451:LEU:HD23	2.42	0.54
1:C:400:ILE:O	1:C:400:ILE:CG2	2.56	0.54
1:H:48:ILE:HD13	1:H:479:MSE:HE1	1.89	0.54
1:H:400:ILE:O	1:H:400:ILE:CG2	2.55	0.54
1:A:298:MSE:HG2	1:A:301:ARG:HH21	1.73	0.53
1:C:431:ARG:HG2	1:C:456:MSE:SE	2.58	0.53
1:G:52:ILE:HD11	1:G:396:PHE:HE2	1.74	0.53
1:I:400:ILE:O	1:I:400:ILE:CG2	2.56	0.53
1:D:208:GLU:HG2	1:D:221:ALA:HA	1.90	0.53
1:E:95:MSE:HG2	1:F:99:LEU:CD1	2.38	0.53
1:F:400:ILE:O	1:F:400:ILE:CG2	2.55	0.53
1:H:382:VAL:CG2	1:H:392:PHE:CZ	2.91	0.53
1:C:326:PRO:O	1:C:330:LYS:HG2	2.09	0.53
1:G:48:ILE:HG22	1:G:482:VAL:HG21	1.91	0.53
1:D:119:VAL:HG21	1:D:256:TYR:CZ	2.45	0.52
1:E:435:ASN:HB2	1:E:455:ARG:NH1	2.25	0.52
1:A:119:VAL:HG21	1:A:256:TYR:CZ	2.45	0.52
1:B:52:ILE:HD11	1:B:396:PHE:CE2	2.45	0.52
1:G:400:ILE:O	1:G:400:ILE:CG2	2.57	0.52
1:H:119:VAL:HG21	1:H:256:TYR:CZ	2.45	0.52
1:A:95:MSE:HG2	1:B:99:LEU:HD11	1.91	0.52
1:D:400:ILE:O	1:D:400:ILE:CG2	2.56	0.52
1:F:355:PHE:O	1:F:415:LEU:CD1	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:VAL:HG21	1:G:256:TYR:CZ	2.45	0.52
1:A:95:MSE:HG2	1:B:99:LEU:CD1	2.40	0.52
1:E:119:VAL:HG21	1:E:256:TYR:CZ	2.45	0.52
1:E:485:GLU:HA	1:E:488:GLN:HG3	1.91	0.51
1:I:406:GLU:OE2	1:I:424:ARG:HD3	2.10	0.51
1:A:74:ILE:HD13	1:A:511:VAL:CG1	2.41	0.51
1:B:119:VAL:HG21	1:B:256:TYR:CZ	2.45	0.51
1:F:439:ARG:HA	1:F:439:ARG:NE	2.25	0.51
1:F:485:GLU:HA	1:F:488:GLN:HG3	1.92	0.51
1:D:298:MSE:HG2	1:D:301:ARG:HH21	1.76	0.51
1:F:74:ILE:HD13	1:F:511:VAL:CG1	2.41	0.51
1:H:74:ILE:HD13	1:H:511:VAL:CG1	2.41	0.51
1:F:287:LEU:HD22	1:F:514:MSE:HE1	1.93	0.50
1:D:426:PHE:HE2	1:E:213:GLN:NE2	2.08	0.50
1:E:74:ILE:HD13	1:E:511:VAL:CG1	2.40	0.50
1:C:74:ILE:HD13	1:C:511:VAL:CG1	2.41	0.50
1:G:74:ILE:HD13	1:G:511:VAL:CG1	2.40	0.50
1:I:485:GLU:HA	1:I:488:GLN:HG3	1.94	0.50
1:C:384:SER:OG	1:C:388:LEU:O	2.29	0.50
1:C:485:GLU:HA	1:C:488:GLN:HG3	1.93	0.50
1:E:461:TYR:OH	1:E:464:VAL:HG13	2.12	0.50
1:E:74:ILE:HA	1:E:511:VAL:HG12	1.94	0.50
1:B:74:ILE:HD13	1:B:511:VAL:CG1	2.42	0.49
1:D:74:ILE:HD13	1:D:511:VAL:CG1	2.41	0.49
1:H:485:GLU:HA	1:H:488:GLN:HG3	1.93	0.49
1:I:74:ILE:HD13	1:I:511:VAL:CG1	2.41	0.49
1:I:194:TYR:CE1	1:I:234:GLU:HG3	2.47	0.49
1:D:485:GLU:HA	1:D:488:GLN:HG3	1.94	0.49
1:B:371:PRO:HG3	1:B:457:SER:HB3	1.94	0.49
1:E:487:LEU:HD11	1:E:511:VAL:HG23	1.94	0.49
1:B:74:ILE:HA	1:B:511:VAL:HG12	1.93	0.49
1:B:498:PHE:O	1:B:502:VAL:HG23	2.13	0.49
1:F:487:LEU:HD11	1:F:511:VAL:HG23	1.95	0.49
1:C:119:VAL:HG21	1:C:256:TYR:CZ	2.48	0.49
1:C:371:PRO:HG3	1:C:457:SER:HB3	1.95	0.49
1:F:382:VAL:CG2	1:F:392:PHE:CZ	2.91	0.49
1:G:485:GLU:HA	1:G:488:GLN:HG3	1.95	0.49
1:A:485:GLU:HA	1:A:488:GLN:HG3	1.93	0.49
1:I:402:TYR:OH	1:I:436:LEU:HD13	2.13	0.49
1:A:74:ILE:HA	1:A:511:VAL:HG12	1.95	0.49
1:B:485:GLU:HA	1:B:488:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:VAL:HG21	1:I:256:TYR:CZ	2.47	0.49
1:A:99:LEU:HD11	1:C:95:MSE:HG2	1.95	0.49
1:H:371:PRO:HG3	1:H:457:SER:HB3	1.94	0.49
1:F:498:PHE:O	1:F:502:VAL:HG23	2.13	0.48
1:I:384:SER:OG	1:I:388:LEU:O	2.29	0.48
1:E:384:SER:OG	1:E:388:LEU:O	2.29	0.48
1:G:287:LEU:HD22	1:G:514:MSE:HE1	1.94	0.48
1:F:119:VAL:HG21	1:F:256:TYR:CZ	2.48	0.48
1:H:498:PHE:O	1:H:502:VAL:HG23	2.13	0.48
1:C:498:PHE:O	1:C:502:VAL:HG23	2.13	0.48
1:A:498:PHE:O	1:A:502:VAL:HG23	2.13	0.48
1:H:355:PHE:O	1:H:415:LEU:CD1	2.61	0.48
1:I:402:TYR:CE1	1:I:436:LEU:CD2	2.91	0.48
1:E:287:LEU:HD22	1:E:514:MSE:HE1	1.95	0.48
1:H:74:ILE:HA	1:H:511:VAL:HG12	1.95	0.48
1:G:498:PHE:O	1:G:502:VAL:HG23	2.13	0.48
1:C:494:GLY:O	1:C:499:GLN:NE2	2.44	0.48
1:D:287:LEU:HD22	1:D:514:MSE:HE1	1.95	0.48
1:E:372:TRP:CH2	1:E:451:LEU:HA	2.49	0.48
1:E:498:PHE:O	1:E:502:VAL:HG23	2.14	0.48
1:G:74:ILE:HA	1:G:511:VAL:HG12	1.95	0.48
1:A:287:LEU:HD22	1:A:514:MSE:HE1	1.96	0.47
1:A:427:ARG:HH21	1:A:431:ARG:NH1	2.12	0.47
1:C:287:LEU:HD22	1:C:514:MSE:HE1	1.95	0.47
1:F:298:MSE:HG2	1:F:301:ARG:NH2	2.30	0.47
1:I:74:ILE:HA	1:I:511:VAL:HG12	1.95	0.47
1:C:298:MSE:HG2	1:C:301:ARG:NH2	2.29	0.47
1:G:95:MSE:HG2	1:H:99:LEU:CD1	2.44	0.47
1:I:498:PHE:O	1:I:502:VAL:HG23	2.13	0.47
1:F:371:PRO:HG3	1:F:457:SER:HB3	1.96	0.47
1:D:74:ILE:HA	1:D:511:VAL:HG12	1.96	0.47
1:D:498:PHE:O	1:D:502:VAL:HG23	2.14	0.47
1:F:74:ILE:HA	1:F:511:VAL:HG12	1.95	0.47
1:D:99:LEU:HD11	1:F:95:MSE:HG2	1.97	0.47
1:H:365:ILE:HG12	1:H:382:VAL:HG12	1.97	0.47
1:C:74:ILE:HA	1:C:511:VAL:HG12	1.96	0.47
1:H:53:GLN:HB3	1:H:489:LYS:HB2	1.97	0.47
1:B:353:GLN:HG3	1:C:200:ALA:O	2.14	0.47
1:B:402:TYR:CE2	1:B:436:LEU:CD2	2.98	0.47
1:F:51:ILE:HG13	1:F:51:ILE:O	2.15	0.46
1:D:461:TYR:OH	1:D:464:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:SER:HB2	1:F:110:ILE:HG12	1.97	0.46
1:A:80:GLY:O	1:A:277:LYS:HD2	2.16	0.46
1:D:80:GLY:O	1:D:277:LYS:HD2	2.16	0.46
1:D:487:LEU:HD11	1:D:511:VAL:HG23	1.98	0.46
1:G:48:ILE:HB	1:G:405:TYR:HB3	1.97	0.46
1:B:80:GLY:O	1:B:277:LYS:HD2	2.16	0.46
1:I:287:LEU:HD22	1:I:514:MSE:HE1	1.98	0.46
1:B:135:SER:HB2	1:C:110:ILE:HG12	1.96	0.46
1:E:80:GLY:O	1:E:277:LYS:HD2	2.15	0.46
1:C:357:VAL:HG22	1:C:413:HIS:CG	2.51	0.46
1:H:80:GLY:O	1:H:277:LYS:HD2	2.16	0.46
1:D:384:SER:OG	1:D:388:LEU:O	2.29	0.46
1:G:373:ASP:HA	1:H:495:PRO:HA	1.98	0.46
1:G:487:LEU:HD11	1:G:511:VAL:HG23	1.98	0.46
1:A:116:ASN:O	1:A:119:VAL:HG22	2.16	0.46
1:D:95:MSE:HG2	1:E:99:LEU:HD11	1.97	0.45
1:A:403:VAL:HG13	1:A:482:VAL:HG23	1.98	0.45
1:B:95:MSE:HG2	1:C:99:LEU:CD1	2.46	0.45
1:C:316:GLU:O	1:C:320:MSE:HG2	2.16	0.45
1:E:298:MSE:HG2	1:E:301:ARG:NH2	2.31	0.45
1:G:80:GLY:O	1:G:277:LYS:HD2	2.16	0.45
1:G:116:ASN:O	1:G:119:VAL:HG22	2.17	0.45
1:H:298:MSE:HG2	1:H:301:ARG:HH21	1.81	0.45
1:A:110:ILE:HG12	1:C:135:SER:HB2	1.97	0.45
1:B:287:LEU:HD22	1:B:514:MSE:HE1	1.99	0.45
1:H:347:ILE:CG2	1:H:352:VAL:HG11	2.47	0.45
1:B:116:ASN:O	1:B:119:VAL:HG22	2.16	0.45
1:B:141:GLY:O	1:B:144:GLU:HB3	2.16	0.45
1:G:52:ILE:CD1	1:G:396:PHE:CE2	2.99	0.45
1:I:80:GLY:O	1:I:277:LYS:HD2	2.17	0.45
1:A:48:ILE:HB	1:A:405:TYR:HB3	1.97	0.45
1:B:459:PRO:O	1:C:213:GLN:NE2	2.50	0.45
1:D:116:ASN:O	1:D:119:VAL:HG22	2.17	0.45
1:F:357:VAL:HG22	1:F:413:HIS:CG	2.52	0.45
1:G:99:LEU:HD11	1:I:95:MSE:HG2	1.98	0.45
1:I:487:LEU:HD11	1:I:511:VAL:HG23	1.98	0.45
1:A:372:TRP:CH2	1:A:451:LEU:HA	2.51	0.45
1:B:358:PRO:HA	1:C:208:GLU:OE1	2.16	0.45
1:F:365:ILE:HG12	1:F:382:VAL:HG12	1.99	0.45
1:I:357:VAL:HG22	1:I:413:HIS:CG	2.52	0.45
1:B:52:ILE:HG23	1:B:488:GLN:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:VAL:HG22	1:B:413:HIS:CG	2.52	0.45
1:C:357:VAL:HG23	1:C:415:LEU:HD12	1.97	0.45
1:C:487:LEU:HD11	1:C:511:VAL:HG23	1.98	0.45
1:D:95:MSE:HG2	1:E:99:LEU:CD1	2.46	0.45
1:E:116:ASN:O	1:E:119:VAL:HG22	2.17	0.45
1:F:347:ILE:CG2	1:F:352:VAL:HG11	2.46	0.45
1:D:461:TYR:OH	1:D:464:VAL:CG2	2.64	0.45
1:F:80:GLY:O	1:F:277:LYS:HD2	2.17	0.45
1:G:52:ILE:CD1	1:G:396:PHE:HE2	2.30	0.45
1:G:365:ILE:HG12	1:G:382:VAL:HG12	1.99	0.45
1:H:357:VAL:HG22	1:H:413:HIS:CG	2.52	0.45
1:I:298:MSE:HG2	1:I:301:ARG:NH2	2.31	0.45
1:A:316:GLU:O	1:A:320:MSE:HG2	2.17	0.44
1:C:371:PRO:CG	1:C:457:SER:HB3	2.47	0.44
1:E:357:VAL:HG22	1:E:413:HIS:CG	2.52	0.44
1:H:116:ASN:O	1:H:119:VAL:HG22	2.17	0.44
1:A:135:SER:HB2	1:B:110:ILE:HG12	1.99	0.44
1:F:52:ILE:HG23	1:F:488:GLN:HB3	2.00	0.44
1:G:99:LEU:CD1	1:I:95:MSE:HG2	2.47	0.44
1:I:347:ILE:CG2	1:I:352:VAL:HG11	2.47	0.44
1:G:141:GLY:O	1:G:144:GLU:HB3	2.17	0.44
1:H:141:GLY:O	1:H:144:GLU:HB3	2.17	0.44
1:H:173:ALA:O	1:H:177:ARG:HG3	2.16	0.44
1:I:427:ARG:HH21	1:I:431:ARG:NH1	2.15	0.44
1:C:141:GLY:O	1:C:144:GLU:HB3	2.17	0.44
1:C:456:MSE:HG2	1:C:457:SER:N	2.32	0.44
1:E:316:GLU:O	1:E:320:MSE:HG2	2.17	0.44
1:G:316:GLU:O	1:G:320:MSE:HG2	2.16	0.44
1:G:357:VAL:HG22	1:G:413:HIS:CG	2.52	0.44
1:A:357:VAL:HG22	1:A:413:HIS:CG	2.52	0.44
1:D:110:ILE:HG12	1:F:135:SER:HB2	1.99	0.44
1:E:427:ARG:HH21	1:E:431:ARG:NH1	2.15	0.44
1:F:87:PRO:O	1:F:367:ILE:HG21	2.17	0.44
1:C:87:PRO:O	1:C:367:ILE:HG21	2.18	0.44
1:D:357:VAL:HG22	1:D:413:HIS:CG	2.53	0.44
1:G:403:VAL:HG13	1:G:482:VAL:HG23	1.98	0.44
1:H:54:GLY:CA	1:H:489:LYS:HG3	2.45	0.44
1:H:95:MSE:HG2	1:I:99:LEU:CD1	2.48	0.44
1:A:99:LEU:CD1	1:C:95:MSE:HG2	2.48	0.44
1:D:427:ARG:HH21	1:D:431:ARG:NH1	2.15	0.44
1:E:141:GLY:O	1:E:144:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ILE:CG2	1:E:352:VAL:HG11	2.48	0.44
1:E:384:SER:HB2	1:E:385:PRO:HD2	2.00	0.44
1:E:489:LYS:HA	1:E:489:LYS:HD3	1.69	0.44
1:F:316:GLU:O	1:F:320:MSE:HG2	2.17	0.44
1:G:427:ARG:HH21	1:G:431:ARG:NH1	2.15	0.44
1:H:287:LEU:HD22	1:H:514:MSE:HE1	1.99	0.44
1:D:95:MSE:HE1	1:E:92:GLU:HG3	2.00	0.44
1:A:371:PRO:HG2	1:A:454:SER:CA	2.46	0.44
1:B:347:ILE:CG2	1:B:352:VAL:HG11	2.48	0.44
1:E:357:VAL:HG23	1:E:415:LEU:HD12	2.00	0.44
1:F:484:ASP:O	1:F:488:GLN:HG3	2.18	0.43
1:H:403:VAL:HG13	1:H:482:VAL:HG23	2.00	0.43
1:C:80:GLY:O	1:C:277:LYS:HD2	2.17	0.43
1:D:141:GLY:O	1:D:144:GLU:HB3	2.18	0.43
1:D:316:GLU:O	1:D:320:MSE:HG2	2.17	0.43
1:A:141:GLY:O	1:A:144:GLU:HB3	2.18	0.43
1:C:427:ARG:O	1:C:431:ARG:HG3	2.19	0.43
1:D:403:VAL:HG13	1:D:482:VAL:HG23	1.99	0.43
1:E:403:VAL:HG13	1:E:482:VAL:HG23	2.01	0.43
1:B:484:ASP:O	1:B:488:GLN:HG3	2.18	0.43
1:I:141:GLY:O	1:I:144:GLU:HB3	2.18	0.43
1:I:357:VAL:HG23	1:I:415:LEU:HD12	1.99	0.43
1:B:403:VAL:HG13	1:B:482:VAL:HG23	2.01	0.43
1:B:487:LEU:HD11	1:B:511:VAL:HG23	2.00	0.43
1:H:487:LEU:HD11	1:H:511:VAL:HG23	2.00	0.43
1:A:492:LEU:HA	1:A:499:GLN:HG2	2.00	0.43
1:C:435:ASN:O	1:C:439:ARG:HG2	2.18	0.43
1:H:430:TYR:HE1	1:H:456:MSE:CE	2.32	0.43
1:I:403:VAL:HG13	1:I:482:VAL:HG23	1.99	0.43
1:A:484:ASP:O	1:A:488:GLN:HG3	2.19	0.43
1:E:298:MSE:HG2	1:E:301:ARG:HH21	1.84	0.43
1:E:492:LEU:HA	1:E:499:GLN:HG2	2.00	0.43
1:F:116:ASN:O	1:F:119:VAL:HG22	2.19	0.43
1:F:141:GLY:O	1:F:144:GLU:HB3	2.18	0.43
1:B:130:VAL:HG13	1:B:150:MSE:HE1	2.01	0.43
1:F:439:ARG:HA	1:F:439:ARG:CZ	2.48	0.43
1:F:494:GLY:O	1:F:499:GLN:NE2	2.51	0.43
1:B:95:MSE:HG2	1:C:99:LEU:HD11	2.01	0.43
1:C:484:ASP:O	1:C:488:GLN:HG3	2.19	0.43
1:F:52:ILE:CD1	1:F:403:VAL:HB	2.49	0.43
1:F:435:ASN:O	1:F:439:ARG:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:LEU:HA	1:G:499:GLN:HG2	2.00	0.43
1:H:87:PRO:O	1:H:367:ILE:HG21	2.19	0.42
1:I:489:LYS:HA	1:I:489:LYS:HD3	1.72	0.42
1:A:48:ILE:CG2	1:A:482:VAL:HG21	2.49	0.42
1:B:87:PRO:O	1:B:367:ILE:HG21	2.19	0.42
1:B:384:SER:HB2	1:B:385:PRO:HD2	2.02	0.42
1:C:116:ASN:O	1:C:119:VAL:HG22	2.19	0.42
1:C:347:ILE:CG2	1:C:352:VAL:HG11	2.48	0.42
1:D:492:LEU:HA	1:D:499:GLN:HG2	2.01	0.42
1:E:171:LYS:HE2	1:E:190:MSE:HE1	2.02	0.42
1:F:371:PRO:CG	1:F:457:SER:HB3	2.50	0.42
1:G:484:ASP:O	1:G:488:GLN:HG3	2.19	0.42
1:H:53:GLN:H	1:H:488:GLN:HB2	1.83	0.42
1:B:316:GLU:O	1:B:320:MSE:HG2	2.19	0.42
1:E:461:TYR:OH	1:E:464:VAL:CG1	2.68	0.42
1:I:316:GLU:O	1:I:320:MSE:HG2	2.19	0.42
1:I:484:ASP:O	1:I:488:GLN:HG3	2.20	0.42
1:G:135:SER:HB2	1:H:110:ILE:HG12	2.02	0.42
1:A:298:MSE:HG2	1:A:301:ARG:NH2	2.35	0.42
1:B:52:ILE:CD1	1:B:396:PHE:CE2	3.03	0.42
1:D:384:SER:HB2	1:D:385:PRO:HD2	2.02	0.42
1:E:152:GLU:HG2	1:E:325:LEU:HD21	2.02	0.42
1:C:130:VAL:HG13	1:C:150:MSE:HE1	2.01	0.42
1:D:332:ILE:HD11	1:D:347:ILE:HG12	2.01	0.42
1:F:152:GLU:HG2	1:F:325:LEU:HD21	2.01	0.42
1:H:316:GLU:O	1:H:320:MSE:HG2	2.20	0.42
1:A:487:LEU:HD11	1:A:511:VAL:HG23	2.01	0.42
1:B:171:LYS:HE2	1:B:190:MSE:HE1	2.02	0.42
1:D:484:ASP:O	1:D:488:GLN:HG3	2.20	0.42
1:H:298:MSE:HG2	1:H:301:ARG:NH2	2.35	0.42
1:H:484:ASP:O	1:H:488:GLN:HG3	2.19	0.42
1:H:494:GLY:O	1:H:499:GLN:NE2	2.53	0.42
1:C:282:THR:O	1:C:286:ILE:HG12	2.20	0.41
1:F:282:THR:O	1:F:286:ILE:HG12	2.20	0.41
1:A:52:ILE:HB	1:A:401:GLU:O	2.20	0.41
1:G:332:ILE:HD11	1:G:347:ILE:HG12	2.02	0.41
1:H:358:PRO:HA	1:I:208:GLU:OE1	2.20	0.41
1:I:87:PRO:O	1:I:367:ILE:HG21	2.21	0.41
1:I:116:ASN:O	1:I:119:VAL:HG22	2.19	0.41
1:I:492:LEU:HA	1:I:499:GLN:HG2	2.01	0.41
1:A:384:SER:HB2	1:A:385:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:347:ILE:CG2	1:G:352:VAL:HG11	2.51	0.41
1:E:282:THR:O	1:E:286:ILE:HG12	2.20	0.41
1:F:52:ILE:HD11	1:F:396:PHE:CE2	2.55	0.41
1:G:87:PRO:O	1:G:367:ILE:HG21	2.21	0.41
1:G:424:ARG:HH21	1:G:429:ALA:HA	1.85	0.41
1:H:130:VAL:HG13	1:H:150:MSE:HE1	2.02	0.41
1:I:282:THR:O	1:I:286:ILE:HG12	2.20	0.41
1:A:332:ILE:HD11	1:A:347:ILE:HG12	2.02	0.41
1:A:347:ILE:CG2	1:A:352:VAL:HG11	2.50	0.41
1:B:324:ILE:HG12	1:B:415:LEU:HD23	2.03	0.41
1:E:434:PHE:CD2	1:E:455:ARG:HA	2.56	0.41
1:H:282:THR:O	1:H:286:ILE:HG12	2.21	0.41
1:I:152:GLU:HG2	1:I:325:LEU:HD21	2.03	0.41
1:A:371:PRO:HG2	1:A:454:SER:CB	2.50	0.41
1:C:171:LYS:HE2	1:C:190:MSE:HE1	2.01	0.41
1:G:357:VAL:HG23	1:G:415:LEU:HD12	2.01	0.41
1:H:152:GLU:HG2	1:H:325:LEU:HD21	2.02	0.41
1:B:371:PRO:CG	1:B:457:SER:HB3	2.51	0.41
1:G:171:LYS:HE2	1:G:190:MSE:HE1	2.02	0.41
1:H:95:MSE:HG2	1:I:99:LEU:HD11	2.03	0.41
1:A:384:SER:OG	1:A:388:LEU:O	2.29	0.41
1:A:424:ARG:HH21	1:A:429:ALA:HA	1.86	0.41
1:D:171:LYS:HE2	1:D:190:MSE:HE1	2.03	0.41
1:E:487:LEU:CD1	1:E:511:VAL:HG23	2.51	0.41
1:F:403:VAL:HG13	1:F:482:VAL:HG23	2.02	0.41
1:G:52:ILE:HG23	1:G:488:GLN:HB3	2.03	0.41
1:I:361:GLN:HA	1:I:383:ILE:HD13	2.03	0.41
1:A:368:TYR:HB3	1:A:459:PRO:HB2	2.03	0.41
1:E:437:ALA:HB1	1:E:451:LEU:HD13	2.03	0.41
1:G:400:ILE:HD13	1:G:437:ALA:O	2.20	0.41
1:A:48:ILE:CG2	1:A:482:VAL:CG2	2.99	0.40
1:A:282:THR:O	1:A:286:ILE:HG12	2.21	0.40
1:E:130:VAL:HG13	1:E:150:MSE:HE1	2.02	0.40
1:F:130:VAL:HG13	1:F:150:MSE:HE1	2.02	0.40
1:H:384:SER:HB2	1:H:385:PRO:HD2	2.03	0.40
1:I:171:LYS:HE2	1:I:190:MSE:HE1	2.03	0.40
1:C:403:VAL:HG13	1:C:482:VAL:HG23	2.02	0.40
1:D:377:VAL:HA	1:D:396:PHE:O	2.21	0.40
1:E:250:ARG:HB3	1:E:250:ARG:CZ	2.52	0.40
1:E:484:ASP:O	1:E:488:GLN:HG3	2.20	0.40
1:G:384:SER:HB2	1:G:385:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:VAL:HG13	1:I:150:MSE:HE1	2.02	0.40
1:B:70:LYS:HB2	1:B:490:HIS:CE1	2.56	0.40
1:D:99:LEU:CD1	1:F:95:MSE:HG2	2.51	0.40
1:F:361:GLN:HA	1:F:383:ILE:HD13	2.03	0.40
1:I:384:SER:HB2	1:I:385:PRO:HD2	2.02	0.40
1:A:357:VAL:HG23	1:A:415:LEU:HD12	2.03	0.40
1:D:130:VAL:HG13	1:D:150:MSE:HE1	2.04	0.40
1:G:377:VAL:HA	1:G:396:PHE:O	2.22	0.40
1:A:87:PRO:O	1:A:367:ILE:HG21	2.21	0.40
1:C:377:VAL:HA	1:C:396:PHE:O	2.22	0.40
1:C:384:SER:HB2	1:C:385:PRO:HD2	2.04	0.40
1:D:282:THR:O	1:D:286:ILE:HG12	2.21	0.40
1:E:87:PRO:O	1:E:367:ILE:HG21	2.21	0.40
1:E:377:VAL:HA	1:E:396:PHE:O	2.22	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	447/490 (91%)	432 (97%)	15 (3%)	0	100	100
1	B	434/490 (89%)	421 (97%)	13 (3%)	0	100	100
1	C	433/490 (88%)	423 (98%)	10 (2%)	0	100	100
1	D	428/490 (87%)	413 (96%)	15 (4%)	0	100	100
1	E	438/490 (89%)	426 (97%)	12 (3%)	0	100	100
1	F	433/490 (88%)	419 (97%)	14 (3%)	0	100	100
1	G	432/490 (88%)	415 (96%)	17 (4%)	0	100	100
1	H	434/490 (89%)	423 (98%)	11 (2%)	0	100	100
1	I	429/490 (88%)	414 (96%)	15 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3908/4410 (89%)	3786 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	383/398 (96%)	377 (98%)	6 (2%)	55	83
1	B	372/398 (94%)	365 (98%)	7 (2%)	50	81
1	C	371/398 (93%)	363 (98%)	8 (2%)	45	78
1	D	366/398 (92%)	359 (98%)	7 (2%)	50	81
1	E	375/398 (94%)	367 (98%)	8 (2%)	47	79
1	F	371/398 (93%)	366 (99%)	5 (1%)	61	86
1	G	370/398 (93%)	365 (99%)	5 (1%)	59	85
1	H	371/398 (93%)	361 (97%)	10 (3%)	39	74
1	I	367/398 (92%)	363 (99%)	4 (1%)	65	87
All	All	3346/3582 (93%)	3286 (98%)	60 (2%)	51	82

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	A	209	ARG
1	A	234	GLU
1	A	333	GLU
1	A	382	VAL
1	A	493	ARG
1	B	186	GLU
1	B	209	ARG
1	B	234	GLU
1	B	382	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	424	ARG
1	B	487	LEU
1	B	493	ARG
1	C	186	GLU
1	C	209	ARG
1	C	234	GLU
1	C	333	GLU
1	C	382	VAL
1	C	424	ARG
1	C	487	LEU
1	C	492	LEU
1	D	186	GLU
1	D	209	ARG
1	D	234	GLU
1	D	333	GLU
1	D	382	VAL
1	D	493	ARG
1	D	514	MSE
1	E	180	GLU
1	E	186	GLU
1	E	209	ARG
1	E	234	GLU
1	E	382	VAL
1	E	487	LEU
1	E	493	ARG
1	E	514	MSE
1	F	186	GLU
1	F	209	ARG
1	F	234	GLU
1	F	415	LEU
1	F	456	MSE
1	G	186	GLU
1	G	209	ARG
1	G	234	GLU
1	G	333	GLU
1	G	493	ARG
1	H	177	ARG
1	H	186	GLU
1	H	209	ARG
1	H	234	GLU
1	H	415	LEU
1	H	424	ARG

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Mol	Chain	Res	Type
1	H	487	LEU
1	H	492	LEU
1	H	493	ARG
1	H	514	MSE
1	I	186	GLU
1	I	189	ARG
1	I	382	VAL
1	I	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	404	HIS
1	A	435	ASN
1	B	71	GLN
1	B	490	HIS
1	C	53	GLN
1	D	149	GLN
1	E	404	HIS
1	E	435	ASN
1	F	149	GLN
1	F	218	GLN
1	G	149	GLN
1	G	218	GLN
1	G	404	HIS
1	H	149	GLN
1	H	404	HIS
1	H	499	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	438/490 (89%)	0.51	28 (6%) 25 18	39, 67, 141, 228	0
1	B	428/490 (87%)	0.39	35 (8%) 17 13	36, 60, 105, 157	0
1	C	427/490 (87%)	0.62	31 (7%) 21 15	43, 67, 108, 148	0
1	D	419/490 (85%)	0.46	19 (4%) 38 30	39, 67, 126, 164	0
1	E	429/490 (87%)	0.50	33 (7%) 19 14	35, 68, 131, 181	0
1	F	427/490 (87%)	0.67	40 (9%) 14 10	44, 70, 113, 166	0
1	G	426/490 (86%)	0.57	28 (6%) 24 18	40, 79, 133, 193	0
1	H	428/490 (87%)	0.46	31 (7%) 21 16	37, 65, 112, 152	0
1	I	421/490 (85%)	0.63	29 (6%) 23 16	45, 79, 133, 176	0
All	All	3843/4410 (87%)	0.53	274 (7%) 22 16	35, 69, 125, 228	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	230	ALA	6.5
1	F	48	ILE	5.9
1	E	213	GLN	5.5
1	A	454	SER	5.5
1	B	55	SER	5.4
1	A	490	HIS	5.3
1	H	46	ALA	5.2
1	B	48	ILE	5.1
1	G	437	ALA	5.1
1	E	491	VAL	5.1
1	F	54	GLY	4.8
1	H	213	GLN	4.8
1	B	291	GLY	4.8
1	H	48	ILE	4.7
1	G	421	VAL	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	51	ILE	4.6
1	H	54	GLY	4.5
1	A	52	ILE	4.5
1	F	231	ALA	4.4
1	C	54	GLY	4.4
1	I	375	ASP	4.4
1	H	441	THR	4.3
1	B	211	GLY	4.3
1	C	48	ILE	4.3
1	B	50	GLY	4.3
1	H	51	ILE	4.2
1	A	421	VAL	4.2
1	D	412	TRP	4.1
1	D	437	ALA	4.1
1	B	70	LYS	4.1
1	I	124	GLY	4.0
1	D	421	VAL	3.9
1	H	182	GLU	3.9
1	H	50	GLY	3.9
1	C	240	ALA	3.8
1	C	181	GLU	3.8
1	B	213	GLN	3.7
1	C	441	THR	3.7
1	E	71	GLN	3.7
1	H	70	LYS	3.6
1	I	181	GLU	3.6
1	H	47	THR	3.6
1	I	70	LYS	3.5
1	A	446	ILE	3.5
1	F	416	GLY	3.5
1	C	277	LYS	3.5
1	E	490	HIS	3.5
1	G	46	ALA	3.5
1	G	51	ILE	3.5
1	B	210	GLU	3.5
1	D	490	HIS	3.5
1	F	179	GLU	3.4
1	F	277	LYS	3.4
1	H	491	VAL	3.4
1	F	50	GLY	3.3
1	B	491	VAL	3.3
1	C	50	GLY	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	210	GLU	3.3
1	G	70	LYS	3.3
1	H	217	ILE	3.3
1	G	77	VAL	3.3
1	E	375	ASP	3.3
1	G	438	SER	3.2
1	I	454	SER	3.2
1	H	439	ARG	3.2
1	I	234	GLU	3.2
1	E	455	ARG	3.2
1	E	295	THR	3.2
1	B	490	HIS	3.1
1	A	70	LYS	3.1
1	D	430	TYR	3.1
1	A	375	ASP	3.1
1	A	513	VAL	3.1
1	D	438	SER	3.1
1	H	295	THR	3.1
1	G	277	LYS	3.1
1	C	53	GLN	3.1
1	I	324	ILE	3.1
1	E	290	PRO	3.1
1	F	441	THR	3.1
1	I	159	GLY	3.0
1	A	451	LEU	3.0
1	F	240	ALA	3.0
1	F	49	ASP	3.0
1	F	375	ASP	3.0
1	G	375	ASP	3.0
1	A	51	ILE	3.0
1	E	489	LYS	3.0
1	B	288	ASP	3.0
1	I	290	PRO	3.0
1	I	421	VAL	3.0
1	E	288	ASP	2.9
1	A	388	LEU	2.9
1	H	49	ASP	2.9
1	B	54	GLY	2.9
1	H	210	GLU	2.9
1	E	493	ARG	2.9
1	D	402	TYR	2.9
1	A	491	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	51	ILE	2.9
1	I	492	LEU	2.9
1	F	290	PRO	2.8
1	B	181	GLU	2.8
1	C	490	HIS	2.8
1	B	53	GLN	2.8
1	D	427	ARG	2.8
1	I	437	ALA	2.8
1	F	70	LYS	2.8
1	D	492	LEU	2.8
1	F	415	LEU	2.8
1	D	411	HIS	2.8
1	B	375	ASP	2.8
1	B	493	ARG	2.7
1	C	52	ILE	2.7
1	C	375	ASP	2.7
1	E	70	LYS	2.7
1	E	427	ARG	2.7
1	G	392	PHE	2.7
1	F	124	GLY	2.7
1	C	47	THR	2.7
1	H	240	ALA	2.6
1	B	492	LEU	2.6
1	F	210	GLU	2.6
1	E	446	ILE	2.6
1	G	412	TRP	2.6
1	C	493	ARG	2.6
1	E	405	TYR	2.6
1	E	73	VAL	2.6
1	I	162	VAL	2.6
1	H	375	ASP	2.6
1	G	457	SER	2.6
1	A	449	LYS	2.6
1	C	70	LYS	2.6
1	F	489	LYS	2.6
1	H	482	VAL	2.6
1	F	213	GLN	2.6
1	I	435	ASN	2.6
1	B	489	LYS	2.5
1	D	70	LYS	2.5
1	I	240	ALA	2.5
1	F	189	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	493	ARG	2.5
1	G	411	HIS	2.5
1	A	50	GLY	2.5
1	E	451	LEU	2.5
1	F	181	GLU	2.5
1	G	47	THR	2.5
1	C	189	ARG	2.5
1	F	47	THR	2.5
1	G	400	ILE	2.5
1	D	491	VAL	2.5
1	F	410	GLN	2.5
1	H	76	ASN	2.5
1	B	472	ILE	2.4
1	C	290	PRO	2.4
1	A	302	GLY	2.4
1	C	291	GLY	2.4
1	B	250	ARG	2.4
1	B	427	ARG	2.4
1	C	439	ARG	2.4
1	B	47	THR	2.4
1	B	400	ILE	2.4
1	A	453	ARG	2.4
1	F	168	SER	2.4
1	C	49	ASP	2.4
1	A	455	ARG	2.4
1	C	427	ARG	2.4
1	D	277	LYS	2.4
1	H	492	LEU	2.4
1	A	48	ILE	2.4
1	C	241	GLY	2.4
1	E	439	ARG	2.4
1	B	72	ALA	2.4
1	F	232	ALA	2.3
1	A	194	TYR	2.3
1	F	217	ILE	2.3
1	H	290	PRO	2.3
1	H	291	GLY	2.3
1	E	214	ASP	2.3
1	C	492	LEU	2.3
1	D	457	SER	2.3
1	G	52	ILE	2.3
1	B	290	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	227	VAL	2.3
1	E	433	PHE	2.3
1	B	216	ALA	2.3
1	H	71	GLN	2.3
1	F	323	SER	2.3
1	G	440	SER	2.3
1	C	184	THR	2.3
1	C	106	GLN	2.3
1	I	413	HIS	2.3
1	E	250	ARG	2.3
1	G	493	ARG	2.3
1	I	493	ARG	2.3
1	H	511	VAL	2.3
1	E	291	GLY	2.3
1	H	72	ALA	2.2
1	G	492	LEU	2.2
1	I	277	LYS	2.2
1	B	439	ARG	2.2
1	I	97	HIS	2.2
1	I	412	TRP	2.2
1	A	427	ARG	2.2
1	A	422	THR	2.2
1	A	333	GLU	2.2
1	E	240	ALA	2.2
1	F	297	LEU	2.2
1	D	431	ARG	2.2
1	E	450	ARG	2.2
1	F	177	ARG	2.2
1	H	490	HIS	2.2
1	E	425	THR	2.2
1	F	295	THR	2.2
1	H	440	SER	2.2
1	E	212	LEU	2.2
1	F	289	ALA	2.2
1	H	53	GLN	2.2
1	I	119	VAL	2.2
1	I	322	THR	2.2
1	E	299	LEU	2.2
1	G	75	LEU	2.2
1	G	436	LEU	2.2
1	A	240	ALA	2.2
1	E	206	GLU	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	221	ALA	2.2
1	F	51	ILE	2.1
1	F	120	ILE	2.1
1	C	119	VAL	2.1
1	B	49	ASP	2.1
1	C	292	GLY	2.1
1	E	441	THR	2.1
1	G	441	THR	2.1
1	F	412	TRP	2.1
1	E	431	ARG	2.1
1	I	125	ARG	2.1
1	F	421	VAL	2.1
1	G	407	ASP	2.1
1	F	243	ALA	2.1
1	D	482	VAL	2.1
1	F	162	VAL	2.1
1	A	459	PRO	2.1
1	G	290	PRO	2.1
1	H	250	ARG	2.1
1	B	240	ALA	2.1
1	E	220	ILE	2.1
1	G	217	ILE	2.1
1	D	404	HIS	2.1
1	I	491	VAL	2.1
1	A	297	LEU	2.1
1	C	297	LEU	2.1
1	F	487	LEU	2.1
1	I	297	LEU	2.1
1	G	50	GLY	2.1
1	B	441	THR	2.1
1	C	431	ARG	2.1
1	E	181	GLU	2.1
1	G	364	SER	2.0
1	I	419	GLN	2.0
1	D	283	LEU	2.0
1	I	441	THR	2.0
1	A	49	ASP	2.0
1	B	71	GLN	2.0
1	B	511	VAL	2.0
1	C	491	VAL	2.0
1	F	97	HIS	2.0
1	A	450	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	217	ILE	2.0
1	I	120	ILE	2.0
1	D	425	THR	2.0
1	I	230	ALA	2.0
1	B	182	GLU	2.0
1	C	82	ASP	2.0
1	A	467	TYR	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.