



# Full wwPDB X-ray Structure Validation Report i

Apr 1, 2014 – 09:36 PM BST

PDB ID : 1VTZ  
Title : 1.45 Angstrom Structure of STNV coat protein (half of the capsid, the other half in PDB 3RQV)  
Authors : Lane, S.W.; Dennis, C.A.; Lane, C.L.; Trinh, C.H.; Rizkallah, P.J.; Stockley, P.G.; Phillips, S.E.V.  
Deposited on : 2011-04-28  
Resolution : 1.45 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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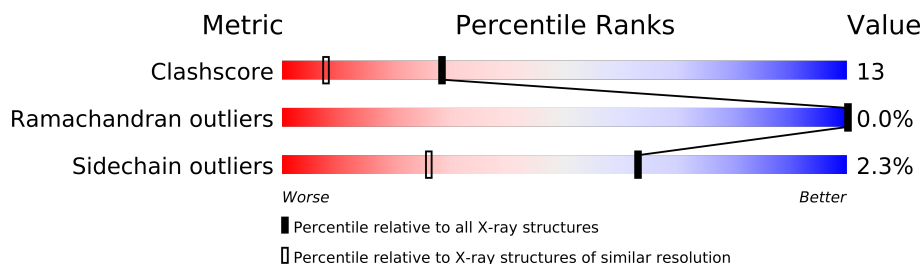
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	<b>NOT EXECUTED</b>
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable23004

# 1 Overall quality at a glance

The reported resolution of this entry is 1.45 Å.



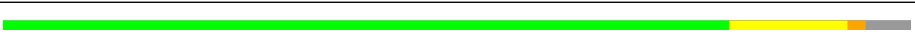












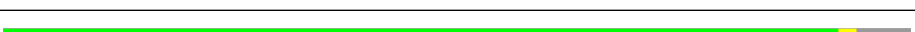
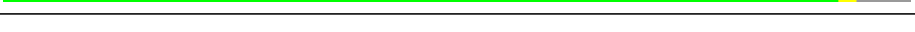
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2834 (1.50-1.42)
Ramachandran outliers	78287	2769 (1.50-1.42)
Sidechain outliers	78261	2767 (1.50-1.42)










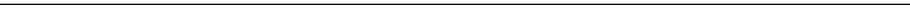

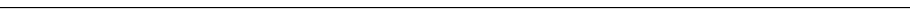
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	0	196	
1	1	196	
1	2	196	
1	3	196	
1	4	196	
1	5	196	
1	6	196	
1	7	196	
1	e	196	
1	f	196	
1	g	196	
1	h	196	
1	i	196	
1	j	196	
1	k	196	
1	l	196	
1	m	196	

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Mol	Chain	Length	Quality of chain
1	n	196	
1	o	196	
1	p	196	
1	q	196	
1	r	196	
1	s	196	
1	t	196	
1	u	196	
1	v	196	
1	w	196	
1	x	196	
1	y	196	
1	z	196	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 51076 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	e	184	Total	C	N	O	S	0	2	0
			1439	898	261	273	7			
1	f	184	Total	C	N	O	S	0	4	0
			1450	908	263	272	7			
1	g	184	Total	C	N	O	S	0	2	0
			1437	898	260	272	7			
1	h	184	Total	C	N	O	S	0	4	0
			1451	906	265	274	6			
1	i	184	Total	C	N	O	S	0	3	0
			1448	902	265	274	7			
1	j	184	Total	C	N	O	S	0	2	0
			1441	898	264	273	6			
1	k	184	Total	C	N	O	S	0	2	0
			1440	897	264	273	6			
1	l	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	m	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	n	184	Total	C	N	O	S	0	4	0
			1450	906	264	273	7			
1	o	184	Total	C	N	O	S	0	1	0
			1433	893	261	273	6			
1	p	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	q	184	Total	C	N	O	S	0	1	0
			1432	893	260	272	7			
1	r	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	s	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	t	184	Total	C	N	O	S	0	7	0
			1472	919	272	274	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	u	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	v	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	w	184	Total	C	N	O	S	0	3	0
			1444	902	263	272	7			
1	x	184	Total	C	N	O	S	0	3	0
			1445	901	264	273	7			
1	y	184	Total	C	N	O	S	0	2	0
			1436	897	260	272	7			
1	z	184	Total	C	N	O	S	0	4	0
			1451	907	264	273	7			
1	0	184	Total	C	N	O	S	0	2	0
			1440	898	263	272	7			
1	1	184	Total	C	N	O	S	0	3	0
			1446	902	264	273	7			
1	2	184	Total	C	N	O	S	0	4	0
			1452	906	266	273	7			
1	3	184	Total	C	N	O	S	0	4	0
			1454	907	267	273	7			
1	4	184	Total	C	N	O	S	0	3	0
			1443	900	262	274	7			
1	5	184	Total	C	N	O	S	0	1	0
			1432	892	261	273	6			
1	6	184	Total	C	N	O	S	0	3	0
			1448	903	266	272	7			
1	7	184	Total	C	N	O	S	0	2	0
			1438	897	261	273	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	g	1	Total	Ca	0	0
			1	1		
2	q	2	Total	Ca	0	0
			2	2		
2	h	1	Total	Ca	0	0
			1	1		
2	6	1	Total	Ca	0	0
			1	1		
2	t	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	o	2	Total 2	Ca 2	0	0
2	2	1	Total 1	Ca 1	0	0
2	y	1	Total 1	Ca 1	0	0
2	f	1	Total 1	Ca 1	0	0
2	p	1	Total 1	Ca 1	0	0
2	k	1	Total 1	Ca 1	0	0
2	w	2	Total 2	Ca 2	0	0
2	n	2	Total 2	Ca 2	0	0
2	5	1	Total 1	Ca 1	0	0
2	x	1	Total 1	Ca 1	0	0
2	s	2	Total 2	Ca 2	0	0
2	j	2	Total 2	Ca 2	0	0
2	1	1	Total 1	Ca 1	0	0
2	e	1	Total 1	Ca 1	0	0
2	v	1	Total 1	Ca 1	0	0
2	4	1	Total 1	Ca 1	0	0
2	r	1	Total 1	Ca 1	0	0
2	m	1	Total 1	Ca 1	0	0
2	0	1	Total 1	Ca 1	0	0
2	i	2	Total 2	Ca 2	0	0
2	7	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	z	1	Total 1	Ca 1	0	0
2	u	1	Total 1	Ca 1	0	0
2	l	1	Total 1	Ca 1	0	0
2	3	1	Total 1	Ca 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	e	259	Total 259	O 259	0	0
3	f	234	Total 234	O 234	0	0
3	g	264	Total 264	O 264	0	0
3	h	278	Total 278	O 278	0	0
3	i	282	Total 282	O 282	0	0
3	j	273	Total 273	O 273	0	0
3	k	253	Total 253	O 253	0	0
3	l	256	Total 256	O 256	0	0
3	m	254	Total 254	O 254	0	0
3	n	253	Total 253	O 253	0	0
3	o	268	Total 268	O 268	0	0
3	p	239	Total 239	O 239	0	0
3	q	254	Total 254	O 254	0	0
3	r	288	Total 288	O 288	0	0
3	s	229	Total 229	O 229	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	t	233	Total 233	O 233	0	0
3	u	231	Total 231	O 231	0	0
3	v	249	Total 249	O 249	0	0
3	w	286	Total 286	O 286	0	0
3	x	259	Total 259	O 259	0	0
3	y	295	Total 295	O 295	0	0
3	z	266	Total 266	O 266	0	0
3	0	245	Total 245	O 245	0	0
3	1	258	Total 258	O 258	0	0
3	2	258	Total 258	O 258	0	0
3	3	245	Total 245	O 245	0	0
3	4	285	Total 285	O 285	0	0
3	5	243	Total 243	O 243	0	0
3	6	265	Total 265	O 265	0	0
3	7	247	Total 247	O 247	0	0



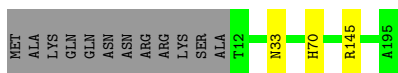
### 3 Residue-property plots

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

Note EDS was not executed.

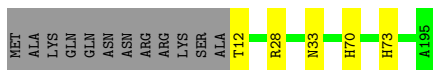
- Molecule 1: Coat protein

Chain e: 



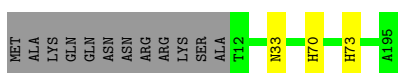
- Molecule 1: Coat protein

Chain f: 



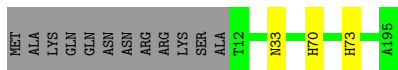
- Molecule 1: Coat protein

Chain g: 



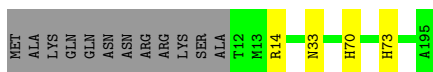
- Molecule 1: Coat protein

Chain h: 



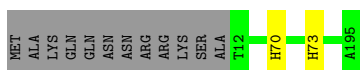
- Molecule 1: Coat protein

Chain i: 



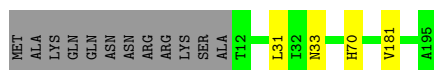
- Molecule 1: Coat protein

Chain j: 



- Molecule 1: Coat protein

Chain s: 



- Molecule 1: Coat protein

Chain t: 



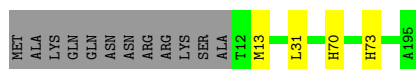
- Molecule 1: Coat protein

Chain u: 



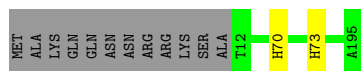
- Molecule 1: Coat protein

Chain v: 



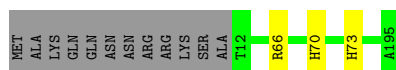
- Molecule 1: Coat protein

Chain w: 



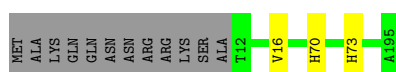
- Molecule 1: Coat protein

Chain x: 



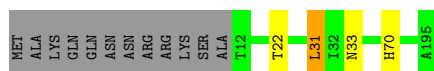
- Molecule 1: Coat protein

Chain y: 



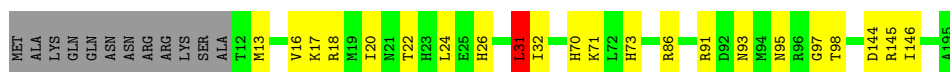
- Molecule 1: Coat protein

Chain z: 



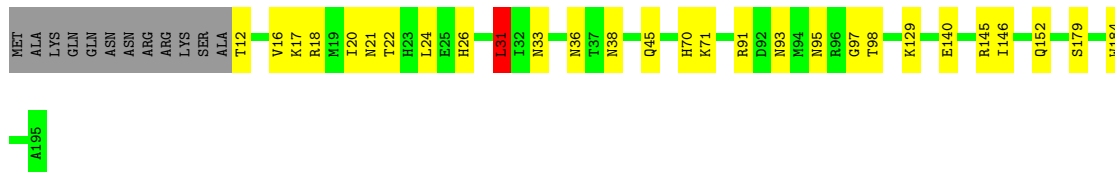
- Molecule 1: Coat protein

Chain 0: 



- Molecule 1: Coat protein

Chain 1:



- Molecule 1: Coat protein

Chain 2:



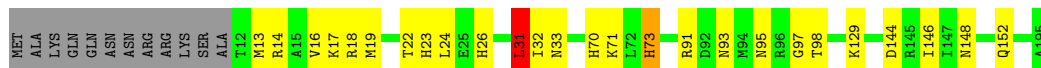
- Molecule 1: Coat protein

Chain 3:



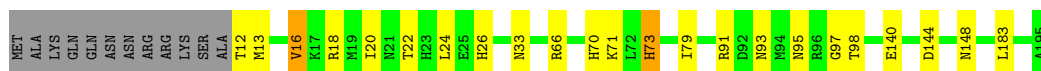
- Molecule 1: Coat protein

Chain 4:



- Molecule 1: Coat protein

Chain 5:



- Molecule 1: Coat protein

Chain 6:



- Molecule 1: Coat protein

Chain 7:



## 4 Data and refinement statistics

EDS was not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	307.58Å 302.26Å 181.92Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	12.00 – 1.45	Depositor
% Data completeness (in resolution range)	99.9 (12.00-1.45)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.175 , 0.208	Depositor
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.059	Xtriage
Estimated twinning fraction	0.007 for k,h,-l 0.009 for -k,-h,-l 0.013 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 2215666 reflections	Xtriage
Total number of atoms	51076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0	0.47	0/1468	0.64	1/1988 (0.1%)
1	1	0.45	0/1477	0.64	1/2000 (0.1%)
1	2	0.45	0/1486	0.62	0/2012
1	3	0.45	0/1488	0.63	1/2014 (0.0%)
1	4	0.46	0/1474	0.62	1/1997 (0.1%)
1	5	0.46	0/1457	0.61	0/1975
1	6	0.44	0/1479	0.62	1/2002 (0.0%)
1	7	0.44	0/1466	0.62	0/1986
1	e	0.46	0/1464	0.64	0/1984
1	f	0.44	0/1484	0.61	0/2010
1	g	0.44	0/1465	0.62	0/1985
1	h	0.47	0/1485	0.65	0/2012
1	i	0.45	0/1476	0.61	0/1999
1	j	0.45	0/1469	0.63	0/1990
1	k	0.48	0/1468	0.64	0/1989
1	l	0.46	0/1457	0.64	1/1974 (0.1%)
1	m	0.43	0/1468	0.60	0/1988
1	n	0.43	0/1484	0.62	0/2010
1	o	0.45	0/1458	0.62	0/1976
1	p	0.45	0/1457	0.64	1/1974 (0.1%)
1	q	0.47	0/1457	0.64	1/1974 (0.1%)
1	r	0.47	0/1479	0.65	1/2002 (0.0%)
1	s	0.46	0/1464	0.63	0/1984
1	t	0.44	0/1515	0.62	1/2050 (0.0%)
1	u	0.46	0/1468	0.61	0/1988
1	v	0.46	0/1468	0.64	0/1988
1	w	0.47	0/1475	0.65	0/1998
1	x	0.46	0/1476	0.63	0/1999
1	y	0.46	0/1464	0.64	0/1984
1	z	0.46	0/1485	0.64	2/2011 (0.1%)
All	All	0.45	0/44181	0.63	12/59843 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	l	31	LEU	CA-CB-CG	6.64	130.58	115.30
1	q	31	LEU	CA-CB-CG	6.54	130.35	115.30
1	p	31	LEU	CA-CB-CG	6.10	129.32	115.30
1	4	31	LEU	CA-CB-CG	5.94	128.96	115.30
1	3	31	LEU	CA-CB-CG	5.89	128.85	115.30
1	t	31	LEU	CA-CB-CG	5.82	128.68	115.30
1	1	31	LEU	CA-CB-CG	5.75	128.52	115.30
1	r	31	LEU	CA-CB-CG	5.54	128.05	115.30
1	6	31	LEU	CA-CB-CG	5.37	127.65	115.30
1	0	31	LEU	CA-CB-CG	5.30	127.50	115.30
1	z	31[A]	LEU	CA-CB-CG	5.10	127.03	115.30
1	z	31[B]	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1440	0	1449	23	0
1	1	1446	0	1457	36	0
1	2	1452	0	1469	57	0
1	3	1454	0	1470	45	0
1	4	1443	0	1450	47	0
1	5	1432	0	1433	36	0
1	6	1448	0	1462	31	0
1	7	1438	0	1444	35	0
1	e	1439	0	1444	0	0
1	f	1450	0	1471	0	0
1	g	1437	0	1447	0	0
1	h	1451	0	1465	0	0
1	i	1448	0	1454	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1441	0	1448	0	0
1	k	1440	0	1446	0	0
1	l	1432	0	1436	0	0
1	m	1440	0	1449	0	0
1	n	1450	0	1466	0	0
1	o	1433	0	1435	0	0
1	p	1432	0	1436	0	0
1	q	1432	0	1436	0	0
1	r	1448	0	1462	0	0
1	s	1436	0	1445	0	0
1	t	1472	0	1502	0	0
1	u	1440	0	1449	0	0
1	v	1440	0	1449	0	0
1	w	1444	0	1458	0	0
1	x	1445	0	1455	0	0
1	y	1436	0	1445	0	0
1	z	1451	0	1468	0	0
2	0	1	0	0	0	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
2	3	1	0	0	0	0
2	4	1	0	0	0	0
2	5	1	0	0	0	0
2	6	1	0	0	0	0
2	7	1	0	0	0	0
2	e	1	0	0	0	0
2	f	1	0	0	0	0
2	g	1	0	0	0	0
2	h	1	0	0	0	0
2	i	2	0	0	0	0
2	j	2	0	0	0	0
2	k	1	0	0	0	0
2	l	1	0	0	0	0
2	m	1	0	0	0	0
2	n	2	0	0	0	0
2	o	2	0	0	0	0
2	p	1	0	0	0	0
2	q	2	0	0	0	0
2	r	1	0	0	0	0
2	s	2	0	0	0	0
2	t	1	0	0	0	0
2	u	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	v	1	0	0	0	0
2	w	2	0	0	0	0
2	x	1	0	0	0	0
2	y	1	0	0	0	0
2	z	1	0	0	0	0
3	0	245	0	0	5	0
3	1	258	0	0	8	0
3	2	258	0	0	7	0
3	3	245	0	0	7	0
3	4	285	0	0	15	2
3	5	243	0	0	2	0
3	6	265	0	0	10	0
3	7	247	0	0	4	0
3	e	259	0	0	0	0
3	f	234	0	0	0	0
3	g	264	0	0	0	0
3	h	278	0	0	0	2
3	i	282	0	0	0	0
3	j	273	0	0	0	0
3	k	253	0	0	0	0
3	l	256	0	0	0	0
3	m	254	0	0	0	0
3	n	253	0	0	0	0
3	o	268	0	0	0	1
3	p	239	0	0	0	0
3	q	254	0	0	0	0
3	r	288	0	0	0	4
3	s	229	0	0	0	0
3	t	233	0	0	0	0
3	u	231	0	0	0	1
3	v	249	0	0	0	0
3	w	286	0	0	0	0
3	x	259	0	0	0	0
3	y	295	0	0	0	0
3	z	266	0	0	0	0
All	All	51076	0	43600	305	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (305) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:7:13:MET:O	1:7:16:VAL:HG12	1.21	1.25
1:2:129:LYS:NZ	1:2:145[A]:ARG:NH2	1.83	1.24
1:2:13:MET:O	1:2:16:VAL:HG13	1.40	1.21
1:2:129:LYS:HZ1	1:2:145[A]:ARG:NH2	1.35	1.16
1:6:13:MET:O	1:6:16:VAL:HG12	1.46	1.12
1:2:13:MET:HA	1:2:16:VAL:CG1	1.79	1.10
1:2:13:MET:O	1:2:16:VAL:CG1	2.00	1.09
1:5:13:MET:O	1:5:16:VAL:CG1	2.02	1.08
1:4:71:LYS:HD3	1:4:148[B]:ASN:HD21	1.19	1.06
1:2:91:ARG:HH11	1:2:93:ASN:HD22	1.04	1.04
1:3:133:LEU:HD21	1:3:145[B]:ARG:HD2	1.39	1.00
1:4:71:LYS:HD3	1:4:148[B]:ASN:ND2	1.73	1.00
1:5:13:MET:O	1:5:16:VAL:HG13	1.60	0.98
1:2:129:LYS:CE	1:2:145[A]:ARG:HH21	1.75	0.98
1:2:17:LYS:HE3	1:2:21:ASN:HD21	1.28	0.97
1:3:91[A]:ARG:HH11	1:3:93:ASN:HD22	1.10	0.97
1:2:17:LYS:HE3	1:2:21:ASN:ND2	1.80	0.96
1:2:129:LYS:NZ	1:2:145[A]:ARG:CZ	2.29	0.95
1:1:91[A]:ARG:NH1	1:1:152:GLN:HB2	1.81	0.95
1:1:18:ARG:HD2	3:1:3037:HOH:O	1.68	0.94
1:3:12:THR:OG1	1:3:15:ALA:HB3	1.68	0.93
1:5:91:ARG:HH11	1:5:93:ASN:HD22	1.10	0.92
1:7:13:MET:O	1:7:16:VAL:CG1	2.15	0.92
1:7:91:ARG:HH11	1:7:93:ASN:HD22	1.14	0.92
1:6:91:ARG:HH11	1:6:93:ASN:HD22	1.13	0.91
1:2:13:MET:HA	1:2:16:VAL:HG11	1.51	0.90
1:6:17:LYS:HB3	3:6:4874:HOH:O	1.70	0.90
1:1:129:LYS:NZ	1:1:145:ARG:HH12	1.69	0.90
1:6:37:THR:HG22	3:6:5143:HOH:O	1.71	0.89
1:4:91:ARG:HH11	1:4:93:ASN:HD22	1.09	0.89
1:1:91[A]:ARG:NH1	3:1:4596:HOH:O	2.06	0.89
1:1:129:LYS:HZ1	1:1:145:ARG:HH12	1.22	0.88
1:1:91[B]:ARG:HE	1:1:93:ASN:ND2	1.71	0.88
1:3:131:VAL:CG1	1:3:145[B]:ARG:HD3	2.04	0.87
1:1:71:LYS:HD2	1:1:146:ILE:HD11	1.55	0.87
1:5:13:MET:O	1:5:16:VAL:HG12	1.72	0.87
1:2:13:MET:CA	1:2:16:VAL:CG1	2.52	0.86
1:2:129:LYS:NZ	1:2:145[A]:ARG:HH21	1.64	0.85
1:4:91:ARG:HH11	1:4:93:ASN:ND2	1.74	0.85
1:0:71:LYS:HD3	1:0:146:ILE:HD11	1.59	0.85
1:2:129:LYS:HZ1	1:2:145[A]:ARG:CZ	1.89	0.84
1:3:13:MET:O	1:3:16:VAL:CG1	2.26	0.84
1:6:13:MET:O	1:6:16:VAL:CG1	2.24	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:129:LYS:CE	1:2:145[A]:ARG:NH2	2.37	0.84
1:2:19:MET:O	1:2:22[B]:THR:HG22	1.77	0.83
1:4:17:LYS:HG2	3:4:3586:HOH:O	1.78	0.83
1:3:13:MET:O	1:3:16:VAL:HG13	1.77	0.83
1:6:91:ARG:HH11	1:6:93:ASN:ND2	1.75	0.83
1:7:91:ARG:HH11	1:7:93:ASN:ND2	1.76	0.83
1:2:91:ARG:HH11	1:2:93:ASN:ND2	1.77	0.82
1:1:45[B]:GLN:HG3	3:1:4039:HOH:O	1.78	0.82
1:3:13:MET:HA	1:3:16:VAL:CG1	2.10	0.81
1:5:91:ARG:HH11	1:5:93:ASN:ND2	1.78	0.81
1:2:95:ASN:HD21	1:2:98:THR:H	1.29	0.80
1:2:129:LYS:HE3	1:2:145[A]:ARG:HH21	1.46	0.80
1:3:95:ASN:HD21	1:3:98:THR:H	1.28	0.80
1:2:131:VAL:HG21	1:2:145[A]:ARG:HD3	1.62	0.80
1:0:91[A]:ARG:HH11	1:0:93:ASN:HD22	1.27	0.79
1:0:91[A]:ARG:HH11	1:0:93:ASN:ND2	1.79	0.79
1:4:13:MET:C	1:4:16:VAL:HG12	2.03	0.79
1:6:28[A]:ARG:HD2	3:6:2454:HOH:O	1.83	0.78
1:3:13:MET:HA	1:3:16:VAL:HG12	1.65	0.78
1:2:129:LYS:HZ2	1:2:145[A]:ARG:CZ	1.96	0.78
1:3:133:LEU:CD2	1:3:145[B]:ARG:HD2	2.14	0.77
1:4:13:MET:HA	1:4:16:VAL:CG1	2.15	0.76
1:3:91[A]:ARG:HH11	1:3:93:ASN:ND2	1.83	0.76
1:4:95:ASN:HD21	1:4:98:THR:H	1.34	0.76
1:3:131:VAL:HG13	1:3:145[B]:ARG:HD3	1.66	0.76
1:7:16:VAL:HG13	1:7:17:LYS:N	2.01	0.76
1:6:129:LYS:NZ	1:6:145:ARG:HH21	1.84	0.75
1:6:129:LYS:NZ	1:6:145:ARG:NH2	2.34	0.75
1:4:31:LEU:CD2	3:4:280:HOH:O	2.33	0.75
1:1:95:ASN:HD21	1:1:98:THR:H	1.34	0.75
1:2:13:MET:C	1:2:16:VAL:CG1	2.55	0.75
1:3:131:VAL:HG11	1:3:145[B]:ARG:HD3	1.69	0.75
1:4:17:LYS:HB3	3:4:3586:HOH:O	1.87	0.74
1:3:131:VAL:HG21	1:3:145[A]:ARG:HD3	1.70	0.74
1:0:95:ASN:HD21	1:0:98:THR:H	1.35	0.73
1:0:145:ARG:NH2	3:0:1039:HOH:O	2.18	0.73
1:5:71:LYS:CG	1:5:148[B]:ASN:OD1	2.36	0.73
1:3:133:LEU:HD21	1:3:145[B]:ARG:CD	2.16	0.73
1:5:95:ASN:HD21	1:5:98:THR:H	1.35	0.73
1:2:129:LYS:HZ2	1:2:145[A]:ARG:NE	1.87	0.73
1:6:95:ASN:HD21	1:6:98:THR:H	1.36	0.73
1:6:26:HIS:HE1	3:6:9660:HOH:O	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:3:13:MET:CA	1:3:16:VAL:HG12	2.19	0.72
1:1:91[B]:ARG:HE	1:1:93:ASN:HD21	1.36	0.72
1:4:13:MET:O	1:4:16:VAL:CG1	2.39	0.71
1:1:91[A]:ARG:NH1	1:1:152:GLN:CB	2.53	0.71
1:7:95:ASN:HD21	1:7:98:THR:H	1.38	0.70
1:3:129:LYS:HE3	1:3:145[A]:ARG:HH21	1.55	0.70
1:2:13:MET:HA	1:2:16:VAL:HG12	1.70	0.70
1:7:71:LYS:HG2	1:7:146:ILE:HD11	1.74	0.69
1:0:146:ILE:HD13	3:0:2036:HOH:O	1.93	0.69
1:7:13:MET:C	1:7:13:MET:SD	2.72	0.68
1:3:131:VAL:HG13	1:3:145[B]:ARG:CD	2.23	0.68
1:4:91:ARG:NH1	1:4:93:ASN:HD22	1.87	0.68
1:5:16:VAL:O	1:5:20:ILE:HG13	1.93	0.68
1:6:91:ARG:NH1	1:6:93:ASN:HD22	1.91	0.68
1:4:23:HIS:HE1	1:7:17:LYS:NZ	1.90	0.68
1:2:13:MET:O	1:2:16:VAL:HG12	1.91	0.67
1:5:71:LYS:CB	1:5:148[B]:ASN:OD1	2.43	0.67
1:2:95:ASN:ND2	1:2:97:GLY:H	1.93	0.66
1:1:91[B]:ARG:NE	1:1:93:ASN:HD21	1.92	0.66
1:1:91[A]:ARG:HG2	1:1:93:ASN:ND2	2.11	0.66
1:4:13:MET:HA	1:4:16:VAL:HG11	1.77	0.66
1:2:13:MET:C	1:2:16:VAL:HG13	2.13	0.66
1:7:16:VAL:HG13	1:7:17:LYS:H	1.61	0.65
1:0:16:VAL:HG13	1:2:19:MET:SD	2.37	0.65
1:5:140:GLU:HG2	3:5:5501:HOH:O	1.97	0.65
1:6:28[B]:ARG:NH1	1:6:28[B]:ARG:HG2	2.10	0.65
1:7:72:LEU:O	1:7:146:ILE:HD12	1.96	0.64
1:2:31:LEU:CD2	3:2:3233:HOH:O	2.44	0.64
1:7:71:LYS:HE3	3:7:5275:HOH:O	1.97	0.64
1:2:13:MET:CA	1:2:16:VAL:HG12	2.26	0.64
1:1:26:HIS:HE1	3:1:5177:HOH:O	1.81	0.64
1:2:131:VAL:CG2	1:2:145[A]:ARG:HD3	2.28	0.64
1:4:17:LYS:CG	3:4:3586:HOH:O	2.39	0.64
1:4:13:MET:CA	1:4:16:VAL:HG12	2.28	0.64
1:4:71:LYS:CD	1:4:148[B]:ASN:HD21	2.03	0.64
1:3:13:MET:C	1:3:16:VAL:HG12	2.19	0.63
1:4:13:MET:HA	1:4:16:VAL:HG12	1.80	0.63
1:0:91[A]:ARG:NH1	1:0:93:ASN:HD22	1.96	0.63
1:6:129:LYS:HZ1	1:6:145:ARG:NH2	1.96	0.63
1:3:146:ILE:CD1	3:3:7614:HOH:O	2.46	0.63
1:5:71:LYS:HB2	1:5:148[B]:ASN:OD1	1.98	0.62
1:2:19:MET:O	1:2:22[B]:THR:CG2	2.47	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:5:12:THR:HG23	1:5:13:MET:H	1.65	0.62
1:6:95:ASN:ND2	1:6:97:GLY:H	1.98	0.62
1:7:95:ASN:ND2	1:7:97:GLY:H	1.98	0.62
1:0:13:MET:HA	1:0:16:VAL:HG12	1.80	0.62
1:0:17:LYS:HE3	3:0:1063:HOH:O	1.99	0.62
1:3:95:ASN:ND2	1:3:97:GLY:H	1.98	0.61
1:3:131:VAL:CG1	1:3:145[B]:ARG:CD	2.77	0.61
1:4:17:LYS:CB	3:4:3586:HOH:O	2.47	0.61
1:4:31:LEU:HD21	3:4:280:HOH:O	1.98	0.61
1:4:23:HIS:CD2	3:4:748:HOH:O	2.53	0.61
1:3:131:VAL:CG2	1:3:145[A]:ARG:HD3	2.30	0.61
1:5:91:ARG:NH1	1:5:93:ASN:HD22	1.91	0.61
1:3:146:ILE:HD11	3:3:7614:HOH:O	2.01	0.61
1:4:31:LEU:HD22	3:4:280:HOH:O	1.97	0.61
1:1:95:ASN:ND2	1:1:97:GLY:H	1.99	0.61
1:5:13:MET:C	1:5:16:VAL:HG12	2.22	0.60
1:4:23:HIS:HE1	1:7:17:LYS:HZ2	1.49	0.60
1:6:129:LYS:HZ1	1:6:145:ARG:HH21	1.49	0.60
1:4:152:GLN:NE2	3:4:1183:HOH:O	2.34	0.60
1:5:95:ASN:ND2	1:5:97:GLY:H	2.00	0.60
1:2:26:HIS:HE1	3:2:1852:HOH:O	1.83	0.59
1:1:129:LYS:NZ	1:1:145:ARG:NH1	2.48	0.59
1:6:66[A]:ARG:HG2	3:6:8067:HOH:O	2.03	0.59
1:0:95:ASN:ND2	1:0:97:GLY:H	1.99	0.59
1:7:91:ARG:NH1	1:7:93:ASN:HD22	1.93	0.59
1:4:95:ASN:ND2	1:4:97:GLY:H	2.00	0.59
1:4:13:MET:O	1:4:16:VAL:HG13	2.02	0.59
1:2:13:MET:C	1:2:16:VAL:HG12	2.22	0.59
1:5:12:THR:HG23	1:5:13:MET:N	2.18	0.59
1:3:13:MET:O	1:3:16:VAL:HG12	2.01	0.58
1:3:152:GLN:NE2	3:3:4244:HOH:O	2.35	0.58
1:7:16:VAL:CG1	1:7:17:LYS:H	2.16	0.58
1:7:73:HIS:HB2	1:7:146:ILE:HD13	1.84	0.58
1:2:91:ARG:NH1	1:2:93:ASN:HD22	1.88	0.58
1:7:16:VAL:CG1	1:7:17:LYS:N	2.66	0.58
1:5:71:LYS:HG3	1:5:148[B]:ASN:OD1	2.03	0.58
1:6:28[B]:ARG:HH11	1:6:28[B]:ARG:HG2	1.68	0.58
1:3:66:ARG:CG	3:3:8219:HOH:O	2.50	0.58
1:0:95:ASN:HD22	1:0:97:GLY:H	1.52	0.57
1:1:31:LEU:C	1:1:31:LEU:HD23	2.25	0.57
1:4:13:MET:C	1:4:16:VAL:CG1	2.73	0.57
1:5:13:MET:HA	1:5:16:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:2:31:LEU:HD21	3:2:3233:HOH:O	2.04	0.57
1:2:31:LEU:HD23	1:2:31:LEU:C	2.25	0.56
1:6:31:LEU:HD23	1:6:31:LEU:C	2.26	0.56
1:2:17:LYS:CE	1:2:21:ASN:HD21	2.10	0.56
1:2:66:ARG:NH2	3:2:1239:HOH:O	2.39	0.55
1:6:14:ARG:N	3:6:4754:HOH:O	2.39	0.55
1:4:13:MET:CA	1:4:16:VAL:CG1	2.83	0.55
1:4:13:MET:O	1:4:16:VAL:HG12	2.04	0.55
1:2:91:ARG:HD3	1:2:93:ASN:ND2	2.22	0.55
1:4:71:LYS:CD	1:4:148[B]:ASN:ND2	2.61	0.54
1:0:31:LEU:C	1:0:31:LEU:HD23	2.27	0.54
1:3:13:MET:HA	1:3:16:VAL:HG11	1.86	0.54
1:2:18:ARG:O	1:2:22[A]:THR:HG23	2.08	0.54
1:3:12:THR:O	1:3:16:VAL:HG12	2.08	0.54
1:0:16:VAL:HG13	1:0:17:LYS:N	2.22	0.53
1:2:95:ASN:HD22	1:2:97:GLY:H	1.55	0.53
1:1:95:ASN:HD22	1:1:97:GLY:H	1.57	0.53
1:6:91:ARG:HD2	3:6:7230:HOH:O	2.08	0.53
1:7:12:THR:CG2	1:7:13:MET:N	2.72	0.52
1:6:18:ARG:O	1:6:22:THR:HG23	2.09	0.52
1:2:13:MET:O	1:2:16:VAL:N	2.42	0.52
1:7:18:ARG:O	1:7:22:THR:HG23	2.10	0.52
1:4:91:ARG:HD2	3:4:4092:HOH:O	2.09	0.52
1:4:23:HIS:CE1	1:7:17:LYS:NZ	2.76	0.52
1:6:129:LYS:HZ2	1:6:145:ARG:HH21	1.55	0.52
1:3:91[A]:ARG:HD3	1:3:93:ASN:ND2	2.25	0.52
1:1:24:LEU:O	1:1:26:HIS:HD2	1.94	0.51
1:5:73:HIS:HE1	1:5:144:ASP:OD2	1.93	0.51
1:4:129:LYS:HE2	3:4:1014:HOH:O	2.11	0.51
1:5:71:LYS:HD3	1:5:148[B]:ASN:OD1	2.11	0.51
1:4:26:HIS:HE1	3:4:1982:HOH:O	1.92	0.51
1:2:28[A]:ARG:HD2	3:2:2113:HOH:O	2.11	0.51
1:1:91[A]:ARG:CZ	1:1:152:GLN:HB2	2.41	0.50
1:4:18:ARG:O	1:4:22:THR:HG23	2.11	0.50
1:5:73:HIS:HD2	3:6:2514:HOH:O	1.94	0.50
1:4:23:HIS:CE1	1:7:17:LYS:HZ3	2.30	0.50
1:1:91[B]:ARG:NE	1:1:93:ASN:ND2	2.47	0.50
1:2:129:LYS:HZ2	1:2:145[A]:ARG:HE	1.60	0.50
1:3:95:ASN:HD22	1:3:97:GLY:H	1.60	0.50
1:3:91[A]:ARG:NH1	1:3:93:ASN:HD22	1.93	0.50
1:4:19:MET:O	1:4:23:HIS:HD2	1.94	0.49
1:3:66:ARG:HG2	3:3:8219:HOH:O	2.11	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:6:31:LEU:HD23	1:6:32:ILE:N	2.27	0.49
1:1:91[A]:ARG:HH12	1:1:152:GLN:HB2	1.74	0.49
1:6:129:LYS:HZ2	1:6:145:ARG:NH2	2.11	0.49
1:2:12:THR:O	1:2:16:VAL:HG12	2.13	0.48
1:2:17:LYS:NZ	3:2:906:HOH:O	2.46	0.48
1:6:28[B]:ARG:CG	1:6:28[B]:ARG:HH11	2.25	0.48
1:3:13:MET:C	1:3:16:VAL:CG1	2.81	0.48
1:0:86:ARG:CZ	3:0:2934:HOH:O	2.62	0.48
1:7:12:THR:HG23	1:7:13:MET:N	2.28	0.48
1:5:91:ARG:HD2	3:5:3876:HOH:O	2.14	0.48
1:1:129:LYS:HZ2	1:1:145:ARG:HH12	1.57	0.48
1:5:13:MET:CA	1:5:16:VAL:HG12	2.43	0.48
1:5:18:ARG:O	1:5:22:THR:HG23	2.14	0.48
1:3:31:LEU:C	1:3:31:LEU:HD23	2.34	0.48
1:0:18:ARG:O	1:0:22:THR:HG23	2.13	0.48
1:1:17:LYS:HE3	1:1:21:ASN:HD21	1.79	0.48
1:3:13:MET:CA	1:3:16:VAL:CG1	2.83	0.48
1:7:95:ASN:HD22	1:7:97:GLY:H	1.60	0.48
1:5:12:THR:HG23	1:5:13:MET:HG2	1.95	0.47
1:7:38:ASN:HB3	1:7:179:SER:O	2.14	0.47
1:1:18:ARG:O	1:1:22:THR:HG23	2.14	0.47
1:5:24:LEU:O	1:5:26:HIS:HD2	1.96	0.47
1:2:31:LEU:HD23	1:2:32:ILE:N	2.29	0.47
1:2:73:HIS:HB2	1:2:146:ILE:CD1	2.45	0.47
1:3:91[A]:ARG:HD3	1:3:93:ASN:HD21	1.79	0.47
1:6:28[B]:ARG:NH2	1:6:189:GLU:OE1	2.47	0.47
1:3:133:LEU:HD21	1:3:145[B]:ARG:CG	2.44	0.47
1:0:73:HIS:HE1	1:0:144:ASP:OD2	1.98	0.47
1:1:91[A]:ARG:HH12	1:1:152:GLN:CB	2.25	0.47
1:4:95:ASN:HD22	1:4:97:GLY:H	1.61	0.47
1:2:129:LYS:HZ2	1:2:145[A]:ARG:NH2	1.87	0.47
1:5:95:ASN:HD22	1:5:97:GLY:H	1.60	0.46
1:7:72:LEU:C	1:7:146:ILE:HD12	2.35	0.46
1:6:18:ARG:NH1	3:6:823:HOH:O	2.48	0.46
1:5:71:LYS:CD	1:5:148[B]:ASN:OD1	2.63	0.46
1:3:133:LEU:HD21	1:3:145[B]:ARG:HG3	1.97	0.46
1:7:91:ARG:HD3	1:7:93:ASN:ND2	2.30	0.46
1:2:91:ARG:HD3	1:2:93:ASN:HD21	1.80	0.46
1:2:24:LEU:O	1:2:26:HIS:HD2	1.99	0.46
1:4:146:ILE:HG23	1:4:146:ILE:O	2.15	0.46
1:5:91:ARG:HD3	1:5:93:ASN:ND2	2.31	0.46
1:7:24:LEU:O	1:7:26:HIS:HD2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:24:LEU:O	1:0:26:HIS:HD2	1.99	0.45
1:7:33:ASN:ND2	3:7:6648:HOH:O	2.48	0.45
1:3:73:HIS:HE1	1:3:144:ASP:OD2	2.00	0.45
1:4:31:LEU:HD23	1:4:31:LEU:C	2.37	0.45
1:4:14:ARG:HB3	3:4:4182:HOH:O	2.16	0.45
1:3:24:LEU:O	1:3:26:HIS:HD2	1.99	0.45
1:2:71:LYS:NZ	3:2:3245:HOH:O	2.49	0.45
1:7:28:ARG:HG2	1:7:191:VAL:HG22	1.99	0.45
1:4:31:LEU:HD23	1:4:32:ILE:N	2.32	0.45
1:7:73:HIS:HB2	1:7:146:ILE:CD1	2.47	0.45
1:1:140:GLU:HG2	3:1:2867:HOH:O	2.17	0.44
1:1:16:VAL:O	1:1:20:ILE:HG13	2.17	0.44
1:1:12:THR:O	1:1:16:VAL:HG12	2.17	0.44
1:2:131:VAL:CG2	1:2:145[A]:ARG:CD	2.95	0.44
1:0:17:LYS:HG2	3:0:4660:HOH:O	2.17	0.43
1:2:28[B]:ARG:NH2	1:2:189:GLU:OE1	2.48	0.43
1:3:31:LEU:HD23	1:3:32:ILE:N	2.33	0.43
1:0:13:MET:CA	1:0:16:VAL:HG12	2.45	0.43
1:4:146:ILE:HG22	3:4:2382:HOH:O	2.18	0.43
1:0:31:LEU:HD23	1:0:32:ILE:N	2.34	0.43
1:0:16:VAL:O	1:0:20:ILE:HG13	2.18	0.43
1:5:66:ARG:HH11	1:5:66:ARG:HG3	1.84	0.43
1:2:146:ILE:O	1:2:146:ILE:HG23	2.18	0.43
1:4:146:ILE:HG23	3:4:5048:HOH:O	2.19	0.43
1:6:95:ASN:HD22	1:6:97:GLY:H	1.63	0.43
1:6:17:LYS:HE3	3:6:4998:HOH:O	2.19	0.42
1:5:13:MET:HA	1:5:16:VAL:CG1	2.48	0.42
1:7:91:ARG:HD3	1:7:93:ASN:HD21	1.84	0.42
1:0:13:MET:HA	1:0:16:VAL:CG1	2.48	0.42
1:4:73:HIS:HE1	1:4:144:ASP:OD2	2.02	0.42
1:1:71:LYS:CD	1:1:146:ILE:HD11	2.39	0.42
1:1:45[B]:GLN:NE2	3:1:2911:HOH:O	2.51	0.42
1:7:12:THR:HA	3:7:4843:HOH:O	2.20	0.42
1:1:36:ASN:HB2	1:1:184:TRP:CE2	2.54	0.42
1:3:146:ILE:HD13	3:3:7614:HOH:O	2.17	0.42
1:6:16:VAL:HG13	1:6:17:LYS:H	1.84	0.42
1:1:17:LYS:NZ	3:1:4776:HOH:O	2.54	0.41
1:4:24:LEU:O	1:4:26:HIS:HD2	2.02	0.41
1:1:17:LYS:HE3	1:1:21:ASN:ND2	2.36	0.41
1:5:71:LYS:HD3	1:5:148[B]:ASN:ND2	2.35	0.41
1:3:91[B]:ARG:HD3	3:3:1316:HOH:O	2.21	0.41
1:1:45[B]:GLN:CG	3:1:4039:HOH:O	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:5:12:THR:CG2	1:5:13:MET:H	2.32	0.41
1:1:38:ASN:HB3	1:1:179:SER:O	2.20	0.41
1:2:12:THR:HG23	1:2:12:THR:O	2.20	0.41
1:7:73:HIS:CB	1:7:146:ILE:HD13	2.51	0.41
1:5:79:ILE:HD12	1:5:183:LEU:HG	2.03	0.41
1:5:66:ARG:HG3	1:5:66:ARG:NH1	2.35	0.41
1:7:27:LYS:HE3	3:7:7326:HOH:O	2.21	0.41
1:4:73:HIS:HB2	1:4:146:ILE:HD12	2.03	0.40
1:3:24:LEU:HD22	1:3:195:ALA:HB2	2.03	0.40
1:5:71:LYS:HD3	1:5:148[B]:ASN:HD21	1.87	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:r:3103:HOH:O	3:4:3133:HOH:O[4_545]	1.23	0.97
3:h:5520:HOH:O	3:r:7427:HOH:O[4_555]	1.60	0.60
3:h:4001:HOH:O	3:r:7427:HOH:O[4_555]	1.78	0.42
3:o:501:HOH:O	3:u:6399:HOH:O[2_555]	1.99	0.21
3:r:6858:HOH:O	3:4:3133:HOH:O[4_545]	2.03	0.17

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	1	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	2	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	3	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	4	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	5	183/196 (93%)	179 (98%)	4 (2%)	0	100	100
1	6	185/196 (94%)	180 (97%)	5 (3%)	0	100	100
1	7	184/196 (94%)	179 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	e	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	f	186/196 (95%)	178 (96%)	8 (4%)	0	100	100
1	g	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	h	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
1	i	185/196 (94%)	179 (97%)	5 (3%)	1 (0%)	38	10
1	j	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	k	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	l	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	m	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	n	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
1	o	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	p	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	q	183/196 (93%)	178 (97%)	5 (3%)	0	100	100
1	r	185/196 (94%)	179 (97%)	6 (3%)	0	100	100
1	s	184/196 (94%)	177 (96%)	7 (4%)	0	100	100
1	t	189/196 (96%)	183 (97%)	6 (3%)	0	100	100
1	u	184/196 (94%)	180 (98%)	4 (2%)	0	100	100
1	v	184/196 (94%)	179 (97%)	5 (3%)	0	100	100
1	w	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
1	x	185/196 (94%)	178 (96%)	7 (4%)	0	100	100
1	y	184/196 (94%)	178 (97%)	6 (3%)	0	100	100
1	z	186/196 (95%)	181 (97%)	5 (3%)	0	100	100
All	All	5539/5880 (94%)	5373 (97%)	165 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	i	14	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	0	159/167 (95%)	157 (99%)	2 (1%)	80	52
1	1	160/167 (96%)	157 (98%)	3 (2%)	69	34
1	2	161/167 (96%)	156 (97%)	5 (3%)	52	15
1	3	161/167 (96%)	157 (98%)	4 (2%)	60	23
1	4	160/167 (96%)	156 (98%)	4 (2%)	60	23
1	5	158/167 (95%)	154 (98%)	4 (2%)	60	23
1	6	160/167 (96%)	158 (99%)	2 (1%)	80	52
1	7	159/167 (95%)	155 (98%)	4 (2%)	60	23
1	e	159/167 (95%)	156 (98%)	3 (2%)	69	34
1	f	161/167 (96%)	156 (97%)	5 (3%)	52	15
1	g	159/167 (95%)	156 (98%)	3 (2%)	69	34
1	h	161/167 (96%)	158 (98%)	3 (2%)	69	34
1	i	160/167 (96%)	157 (98%)	3 (2%)	69	34
1	j	159/167 (95%)	157 (99%)	2 (1%)	80	52
1	k	159/167 (95%)	156 (98%)	3 (2%)	69	34
1	l	158/167 (95%)	154 (98%)	4 (2%)	60	23
1	m	159/167 (95%)	155 (98%)	4 (2%)	60	23
1	n	161/167 (96%)	158 (98%)	3 (2%)	69	34
1	o	158/167 (95%)	155 (98%)	3 (2%)	69	34
1	p	158/167 (95%)	154 (98%)	4 (2%)	60	23
1	q	158/167 (95%)	154 (98%)	4 (2%)	60	23
1	r	160/167 (96%)	152 (95%)	8 (5%)	34	5
1	s	159/167 (95%)	154 (97%)	5 (3%)	52	15
1	t	164/167 (98%)	159 (97%)	5 (3%)	53	16
1	u	159/167 (95%)	154 (97%)	5 (3%)	52	15
1	v	159/167 (95%)	155 (98%)	4 (2%)	60	23
1	w	160/167 (96%)	158 (99%)	2 (1%)	80	52
1	x	160/167 (96%)	157 (98%)	3 (2%)	69	34
1	y	159/167 (95%)	156 (98%)	3 (2%)	69	34
1	z	161/167 (96%)	156 (97%)	5 (3%)	52	15
All	All	4789/5010 (96%)	4677 (98%)	112 (2%)	63	26

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	33	ASN
1	e	70	HIS
1	e	145	ARG
1	f	12	THR
1	f	28	ARG
1	f	33	ASN
1	f	70	HIS
1	f	73	HIS
1	g	33	ASN
1	g	70	HIS
1	g	73	HIS
1	h	33	ASN
1	h	70	HIS
1	h	73	HIS
1	i	33	ASN
1	i	70	HIS
1	i	73	HIS
1	j	70	HIS
1	j	73	HIS
1	k	31	LEU
1	k	33	ASN
1	k	70	HIS
1	l	31	LEU
1	l	33	ASN
1	l	70	HIS
1	l	73	HIS
1	m	22	THR
1	m	31	LEU
1	m	33	ASN
1	m	70	HIS
1	n	21	ASN
1	n	22	THR
1	n	70	HIS
1	o	16	VAL
1	o	70	HIS
1	o	73	HIS
1	p	13	MET
1	p	31	LEU
1	p	33	ASN
1	p	70	HIS
1	q	16	VAL
1	q	28	ARG

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Mol	Chain	Res	Type
1	q	31	LEU
1	q	70	HIS
1	r	12	THR
1	r	16	VAL
1	r	31	LEU
1	r	33	ASN
1	r	70	HIS
1	r	73	HIS
1	r	145[A]	ARG
1	r	145[B]	ARG
1	s	31	LEU
1	s	33	ASN
1	s	70	HIS
1	s	181[A]	VAL
1	s	181[B]	VAL
1	t	22	THR
1	t	31	LEU
1	t	33	ASN
1	t	70	HIS
1	t	73	HIS
1	u	16	VAL
1	u	31	LEU
1	u	33	ASN
1	u	70	HIS
1	u	73	HIS
1	v	13	MET
1	v	31	LEU
1	v	70	HIS
1	v	73	HIS
1	w	70	HIS
1	w	73	HIS
1	x	66	ARG
1	x	70	HIS
1	x	73	HIS
1	y	16	VAL
1	y	70	HIS
1	y	73	HIS
1	z	22	THR
1	z	31[A]	LEU
1	z	31[B]	LEU
1	z	33	ASN
1	z	70	HIS

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Mol	Chain	Res	Type
1	0	31	LEU
1	0	70	HIS
1	1	31	LEU
1	1	33	ASN
1	1	70	HIS
1	2	16	VAL
1	2	31	LEU
1	2	33	ASN
1	2	70	HIS
1	2	73	HIS
1	3	31	LEU
1	3	33	ASN
1	3	70	HIS
1	3	73	HIS
1	4	31	LEU
1	4	33	ASN
1	4	70	HIS
1	4	73	HIS
1	5	16	VAL
1	5	33	ASN
1	5	70	HIS
1	5	73	HIS
1	6	31	LEU
1	6	70	HIS
1	7	33	ASN
1	7	70	HIS
1	7	71	LYS
1	7	73	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (239) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	21	ASN
1	e	23	HIS
1	e	26	HIS
1	e	33	ASN
1	e	36	ASN
1	e	73	HIS
1	e	93	ASN
1	e	95	ASN
1	e	134	ASN
1	f	23	HIS

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Mol	Chain	Res	Type
1	f	26	HIS
1	f	33	ASN
1	f	36	ASN
1	f	73	HIS
1	f	93	ASN
1	f	95	ASN
1	f	134	ASN
1	g	23	HIS
1	g	26	HIS
1	g	33	ASN
1	g	36	ASN
1	g	73	HIS
1	g	93	ASN
1	g	95	ASN
1	g	134	ASN
1	g	152	GLN
1	h	23	HIS
1	h	26	HIS
1	h	73	HIS
1	h	93	ASN
1	h	95	ASN
1	h	134	ASN
1	i	23	HIS
1	i	26	HIS
1	i	33	ASN
1	i	36	ASN
1	i	73	HIS
1	i	93	ASN
1	i	95	ASN
1	i	134	ASN
1	j	23	HIS
1	j	26	HIS
1	j	33	ASN
1	j	73	HIS
1	j	93	ASN
1	j	95	ASN
1	j	134	ASN
1	k	26	HIS
1	k	33	ASN
1	k	36	ASN
1	k	73	HIS
1	k	93	ASN

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Mol	Chain	Res	Type
1	k	95	ASN
1	k	134	ASN
1	l	26	HIS
1	l	33	ASN
1	l	36	ASN
1	l	45	GLN
1	l	73	HIS
1	l	93	ASN
1	l	95	ASN
1	l	134	ASN
1	m	21	ASN
1	m	26	HIS
1	m	33	ASN
1	m	36	ASN
1	m	73	HIS
1	m	93	ASN
1	m	95	ASN
1	m	134	ASN
1	n	21	ASN
1	n	26	HIS
1	n	33	ASN
1	n	36	ASN
1	n	73	HIS
1	n	93	ASN
1	n	95	ASN
1	n	134	ASN
1	o	21	ASN
1	o	23	HIS
1	o	26	HIS
1	o	73	HIS
1	o	93	ASN
1	o	95	ASN
1	o	134	ASN
1	p	21	ASN
1	p	23	HIS
1	p	26	HIS
1	p	33	ASN
1	p	36	ASN
1	p	73	HIS
1	p	93	ASN
1	p	95	ASN
1	p	134	ASN

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Mol	Chain	Res	Type
1	q	21	ASN
1	q	23	HIS
1	q	26	HIS
1	q	33	ASN
1	q	36	ASN
1	q	73	HIS
1	q	93	ASN
1	q	95	ASN
1	q	134	ASN
1	q	175	GLN
1	r	21	ASN
1	r	26	HIS
1	r	33	ASN
1	r	36	ASN
1	r	73	HIS
1	r	93	ASN
1	r	95	ASN
1	r	134	ASN
1	s	23	HIS
1	s	26	HIS
1	s	33	ASN
1	s	36	ASN
1	s	73	HIS
1	s	93	ASN
1	s	95	ASN
1	s	134	ASN
1	t	21	ASN
1	t	23	HIS
1	t	26	HIS
1	t	33	ASN
1	t	36	ASN
1	t	45	GLN
1	t	73	HIS
1	t	93	ASN
1	t	95	ASN
1	t	134	ASN
1	u	21	ASN
1	u	23	HIS
1	u	26	HIS
1	u	33	ASN
1	u	36	ASN
1	u	73	HIS

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Mol	Chain	Res	Type
1	u	93	ASN
1	u	95	ASN
1	u	134	ASN
1	v	26	HIS
1	v	33	ASN
1	v	36	ASN
1	v	73	HIS
1	v	93	ASN
1	v	95	ASN
1	v	134	ASN
1	w	26	HIS
1	w	33	ASN
1	w	36	ASN
1	w	73	HIS
1	w	93	ASN
1	w	95	ASN
1	w	134	ASN
1	x	26	HIS
1	x	33	ASN
1	x	36	ASN
1	x	73	HIS
1	x	93	ASN
1	x	95	ASN
1	x	134	ASN
1	x	152	GLN
1	y	21	ASN
1	y	23	HIS
1	y	26	HIS
1	y	33	ASN
1	y	36	ASN
1	y	73	HIS
1	y	93	ASN
1	y	95	ASN
1	y	134	ASN
1	z	21	ASN
1	z	23	HIS
1	z	26	HIS
1	z	33	ASN
1	z	36	ASN
1	z	73	HIS
1	z	93	ASN
1	z	95	ASN

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Mol	Chain	Res	Type
1	z	134	ASN
1	0	23	HIS
1	0	26	HIS
1	0	33	ASN
1	0	36	ASN
1	0	73	HIS
1	0	93	ASN
1	0	95	ASN
1	0	134	ASN
1	1	21	ASN
1	1	26	HIS
1	1	33	ASN
1	1	36	ASN
1	1	73	HIS
1	1	93	ASN
1	1	95	ASN
1	1	134	ASN
1	2	21	ASN
1	2	26	HIS
1	2	33	ASN
1	2	36	ASN
1	2	73	HIS
1	2	93	ASN
1	2	95	ASN
1	2	134	ASN
1	3	23	HIS
1	3	26	HIS
1	3	73	HIS
1	3	93	ASN
1	3	95	ASN
1	3	134	ASN
1	4	23	HIS
1	4	26	HIS
1	4	33	ASN
1	4	36	ASN
1	4	73	HIS
1	4	93	ASN
1	4	95	ASN
1	4	134	ASN
1	5	23	HIS
1	5	26	HIS
1	5	33	ASN

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Mol	Chain	Res	Type
1	5	36	ASN
1	5	73	HIS
1	5	93	ASN
1	5	95	ASN
1	5	134	ASN
1	6	21	ASN
1	6	26	HIS
1	6	33	ASN
1	6	36	ASN
1	6	73	HIS
1	6	93	ASN
1	6	95	ASN
1	6	134	ASN
1	7	26	HIS
1	7	33	ASN
1	7	73	HIS
1	7	93	ASN
1	7	95	ASN
1	7	134	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 37 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.