



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2019 – 10:53 AM EDT

PDB ID : 2Y1V  
Title : Full length structure of RrgB Pilus protein from *Streptococcus pneumoniae*  
Authors : El-Mortaji, L.; Contreras-Martel, C.; Manzano, C.; Vernet, T.; Dessen, A.; DiGuilmi, A.M.  
Deposited on : 2010-12-10  
Resolution : 2.39 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

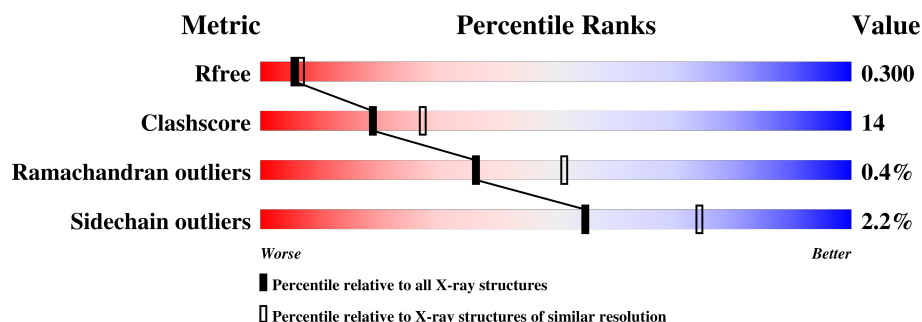
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.39 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	605	 76% 22% .
1	B	605	 77% 22% .
1	C	605	 69% 30% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14167 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 CELL WALL SURFACE ANCHOR FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			
1	B	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			
1	C	604	Total	C	N	O	Se	0	0	0
			4576	2866	763	942	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q97SC2
B	29	GLY	-	expression tag	UNP Q97SC2
C	29	GLY	-	expression tag	UNP Q97SC2

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ni	0	0
			3	3		
2	A	3	Total	Ni	0	0
			3	3		
2	C	3	Total	Ni	0	0
			3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	169	Total	O	0	0
			169	169		
3	B	141	Total	O	0	0
			141	141		

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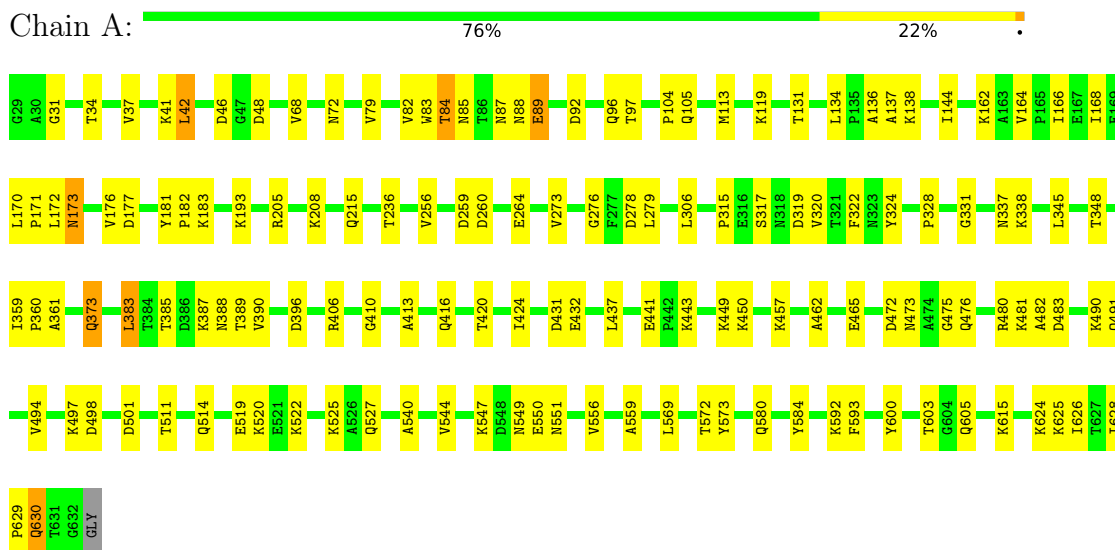
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	120	Total 120	O 120	0	0

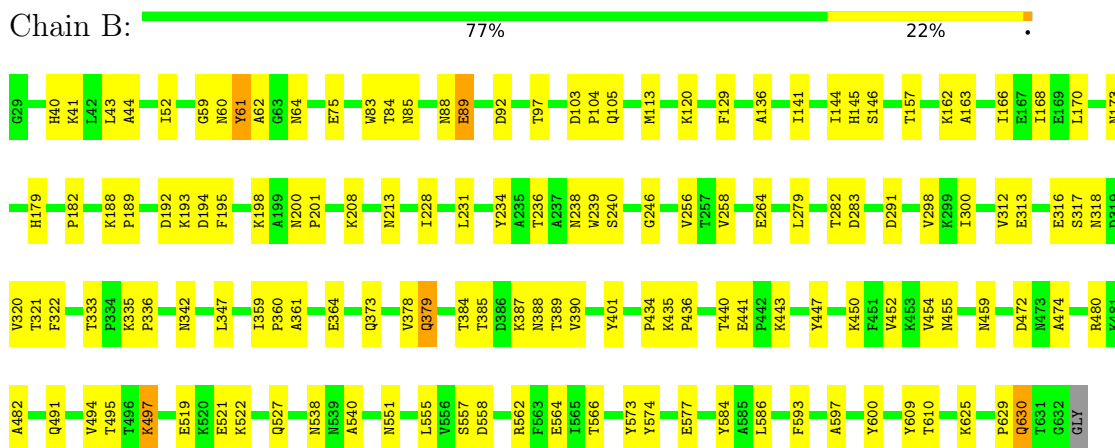
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

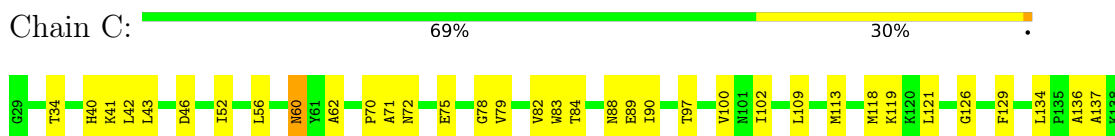
#### • Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



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V254	E405	V493	V494	T495	T496	K497	D498	A499	L500	D501	R502	Y507	L510	E521	A526	Y530	V534	A540	D546	K547	D548	N549	V552	V553	K554	D558	A559	Q560	G561	R562	L569	Y573	E577	P581	A582	G583	L586	S589	F593	Y600	Q605			
V254	E405	V493	V494	T495	T496	K497	D498	A499	L500	D501	R502	Y507	L510	E521	A526	Y530	V534	A540	D546	K547	D548	N549	V552	V553	K554	D558	A559	Q560	G561	R562	L569	Y573	E577	P581	A582	G583	L586	S589	F593	Y600	Q605			
D259	G410	Y411	S412	A413	D414	Y415	Q416	T420	A421	G422	E423	Y426	Y429	E432	N433	P434	D438	E441	P442	K443	K449	K450	F451	Y452	D456	K457	D458	A462	G463	A464	E465	F466	D472	Q476	R480	K481	A482	D483	K484	V485	E489	K490	Q491	L492
D260	Y411	S412	A413	D414	Y415	Q416	T420	A421	G422	E423	Y426	Y429	E432	N433	P434	D438	E441	P442	K443	K449	K450	F451	Y452	D456	K457	D458	A462	G463	A464	E465	F466	D472	Q476	R480	K481	A482	D483	K484	V485	E489	K490	Q491	L492	
E264	A163	V164	P165	I166	E167	I168	F169	L170	V175	V176	D177	A178	H179	V180	Y181	F182	K183	E186	A187	K193	D194	F195	R205	V206	D207	Q215	T224	K227	I228	P229	N233	N238	W239	S240	D241	R242	A248							
L270	T159	G160	S161	K162	A163	V164	P165	I166	E167	I168	F169	L170	V312	E313	S317	N318	D319	V320	T321	F322	N323	Y324	G325	N326	T333	N342	G343	D344	L347	T348	A357	P358	I359	Q373	K376	L383	T384	K387	N388	T389	V390	N393		

T627	T628	P629	Q630	T631	G632	GLY
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.62Å 74.62Å 340.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.53 – 2.39 19.85 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.7 (113.53-2.39) 93.7 (19.85-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.234 0.239 , 0.300	Depositor DCC
$R_{free}$ test set	8066 reflections (10.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.6	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.097 for h,-h-k,-l 0.002 for -k,-h,-l	Xtriage
Reported twinning fraction	0.592 for H, K, L 0.408 for K, H, -L	Depositor
Outliers	0 of 78179 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

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

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	0/4646	0.62	0/6315
1	B	0.44	0/4646	0.57	0/6315
1	C	0.40	0/4646	0.57	0/6315
All	All	0.44	0/13938	0.59	0/18945

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4576	0	4509	108	0
1	B	4576	0	4509	120	0
1	C	4576	0	4510	153	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	169	0	0	12	0
3	B	141	0	0	15	0
3	C	120	0	0	33	0
All	All	14167	0	13528	381	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 14.

All (381) 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:84:THR:HG21	1:B:88:ASN:HA	1.24	1.15
3:A:2008:HOH:O	1:B:387:LYS:HB2	1.45	1.15
1:B:256:VAL:HG21	1:B:279:LEU:HD11	1.16	1.13
1:A:96:GLN:HB3	3:A:2012:HOH:O	1.48	1.12
1:C:168:ILE:HB	3:C:2026:HOH:O	1.47	1.11
1:C:248:ALA:HB3	3:C:2043:HOH:O	1.52	1.06
1:C:312:VAL:HG12	1:C:313:GLU:HG3	1.39	1.04
1:C:82:VAL:CG1	1:C:144:ILE:HD11	1.90	1.01
1:B:240:SER:HB2	3:B:2073:HOH:O	1.59	1.00
1:C:238:ASN:HB3	3:C:2039:HOH:O	1.63	0.98
1:B:84:THR:HG22	1:B:85:ASN:O	1.65	0.94
1:B:256:VAL:CG2	1:B:279:LEU:HD11	1.97	0.93
1:B:521:GLU:HG3	3:B:2117:HOH:O	1.68	0.92
1:A:113:MSE:HE1	1:A:144:ILE:CD1	1.99	0.92
1:B:84:THR:CG2	1:B:88:ASN:HA	1.98	0.92
1:B:256:VAL:HG21	1:B:279:LEU:CD1	2.00	0.92
1:C:491:GLN:O	1:C:494:VAL:HG12	1.70	0.90
1:C:348:THR:HG23	1:C:389:THR:HG22	1.53	0.90
1:C:82:VAL:HG11	1:C:144:ILE:HD11	1.53	0.89
1:C:70:PRO:HA	3:C:2002:HOH:O	1.73	0.88
1:C:464:ALA:HB2	1:C:581:PRO:HD3	1.53	0.87
1:C:416:GLN:HA	3:C:2083:HOH:O	1.76	0.85
1:A:84:THR:HG22	1:A:85:ASN:O	1.77	0.84
1:B:630:GLN:N	1:B:630:GLN:HE21	1.75	0.84
1:A:83:TRP:CH2	1:A:168:ILE:HD11	2.14	0.82
1:B:629:PRO:C	1:B:630:GLN:HE21	1.83	0.82
1:C:546:ASP:OD2	1:C:548:ASP:HB3	1.79	0.82
1:C:449:LYS:NZ	1:C:605:GLN:OE1	2.13	0.82
1:C:82:VAL:HG12	1:C:144:ILE:HD11	1.61	0.80
1:A:511:THR:HG22	1:A:514:GLN:HE21	1.47	0.80
1:C:102:ILE:HG12	1:C:109:LEU:HD12	1.62	0.80
1:C:462:ALA:HB2	1:C:559:ALA:HA	1.63	0.80
1:C:549:ASN:HB3	1:C:552:VAL:HG23	1.62	0.79
1:B:88:ASN:ND2	1:B:104:PRO:HG3	1.98	0.79
1:B:491:GLN:O	1:B:494:VAL:HG12	1.83	0.78
1:C:452:VAL:HA	1:C:561:GLY:O	1.82	0.78
1:A:113:MSE:HE1	1:A:144:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:PRO:C	1:C:630:GLN:HE21	1.91	0.74
1:B:387:LYS:HG3	1:B:387:LYS:O	1.88	0.74
1:B:40:HIS:NE2	1:B:179:HIS:HD2	1.85	0.74
1:C:583:GLY:HA3	3:C:2114:HOH:O	1.87	0.73
1:C:60:ASN:OD1	1:C:62:ALA:O	2.07	0.72
1:C:224:ILE:HD11	1:C:320:VAL:HG21	1.71	0.72
1:A:549:ASN:OD1	1:A:550:GLU:N	2.22	0.72
1:A:416:GLN:HB3	3:A:2102:HOH:O	1.90	0.71
1:A:624:LYS:HG2	3:A:2168:HOH:O	1.92	0.70
1:C:376:LYS:HD2	3:C:2071:HOH:O	1.91	0.70
1:C:423:GLU:O	3:C:2084:HOH:O	2.08	0.70
1:A:82:VAL:HG11	1:A:144:ILE:HD11	1.72	0.70
1:A:84:THR:CG2	1:A:85:ASN:O	2.40	0.69
1:B:92:ASP:OD2	3:B:2013:HOH:O	2.11	0.69
1:A:84:THR:HG21	1:A:88:ASN:HA	1.73	0.69
1:C:489:GLU:OE1	3:C:2091:HOH:O	2.10	0.69
1:C:410:GLY:HA2	1:C:432:GLU:HA	1.76	0.68
1:B:192:ASP:OD1	1:B:208:LYS:NZ	2.24	0.68
1:B:61:TYR:OH	1:B:64:ASN:ND2	2.27	0.67
1:C:348:THR:HG23	1:C:389:THR:CG2	2.24	0.66
1:B:84:THR:CG2	1:B:88:ASN:CA	2.73	0.66
1:C:305:THR:HB	3:C:2043:HOH:O	1.94	0.66
1:B:573:TYR:HB2	1:B:593:PHE:CZ	2.31	0.66
1:C:554:LYS:NZ	3:C:2107:HOH:O	2.29	0.66
1:B:246:GLY:HA3	1:B:316:GLU:CD	2.15	0.65
1:C:82:VAL:CG1	1:C:144:ILE:CD1	2.73	0.65
1:A:603:THR:CG2	1:A:615:LYS:HG2	2.27	0.65
1:A:166:ILE:HG22	1:A:168:ILE:HG23	1.77	0.64
1:B:494:VAL:HG23	3:B:2114:HOH:O	1.96	0.64
1:C:72:ASN:HB3	3:C:2008:HOH:O	1.97	0.64
1:C:83:TRP:CH2	1:C:168:ILE:HD11	2.32	0.64
1:B:256:VAL:CG2	1:B:279:LEU:CD1	2.68	0.64
1:A:387:LYS:O	1:A:387:LYS:CG	2.47	0.63
1:C:238:ASN:CB	3:C:2039:HOH:O	2.30	0.63
1:A:113:MSE:CE	1:A:144:ILE:HD13	2.29	0.62
1:B:146:SER:HB2	3:B:2022:HOH:O	1.99	0.62
1:C:383:LEU:CD1	1:C:390:VAL:HB	2.30	0.62
1:B:480:ARG:HD3	1:B:538:ASN:OD1	2.00	0.62
1:C:319:ASP:HA	1:C:441:GLU:CD	2.20	0.62
1:A:361:ALA:HB3	1:A:385:THR:HG23	1.80	0.62
1:A:476:GLN:HB3	1:A:544:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD13	1:C:279:LEU:HD12	1.83	0.61
1:C:321:THR:HG21	3:C:2088:HOH:O	1.98	0.61
1:C:383:LEU:HD11	1:C:390:VAL:HB	1.82	0.61
1:C:433:ASN:HB3	1:C:434:PRO:CD	2.31	0.61
1:C:90:ILE:HD11	1:C:109:LEU:HD11	1.82	0.61
1:C:82:VAL:HG12	1:C:144:ILE:CD1	2.30	0.61
1:C:558:ASP:OD1	1:C:560:GLN:N	2.30	0.61
1:A:113:MSE:CE	1:A:144:ILE:CD1	2.76	0.61
1:C:41:LYS:HG3	1:C:79:VAL:HG21	1.82	0.61
1:B:519:GLU:OE1	1:B:519:GLU:HA	2.01	0.60
1:B:388:ASN:HA	3:B:2084:HOH:O	2.01	0.60
1:A:42:LEU:HD22	1:A:181:TYR:HB3	1.83	0.60
1:B:387:LYS:C	3:B:2084:HOH:O	2.39	0.60
1:C:242:ARG:NH1	3:C:2041:HOH:O	2.32	0.60
1:A:215:GLN:HB3	1:A:569:LEU:HG	1.83	0.60
1:B:83:TRP:CH2	1:B:168:ILE:HD11	2.37	0.60
1:A:168:ILE:O	1:A:168:ILE:HG13	2.00	0.60
1:C:627:THR:O	1:C:629:PRO:HD3	2.02	0.60
1:B:258:VAL:HG22	1:B:298:VAL:HG22	1.84	0.60
1:C:240:SER:HB2	3:C:2060:HOH:O	2.02	0.60
1:C:241:ASP:HB2	1:C:320:VAL:HG22	1.83	0.59
1:A:603:THR:HG21	1:A:615:LYS:HG2	1.85	0.59
1:B:359:ILE:HB	1:B:360:PRO:HD2	1.84	0.59
1:B:452:VAL:HG12	1:B:454:VAL:HG13	1.84	0.59
1:B:40:HIS:NE2	1:B:179:HIS:CD2	2.69	0.59
1:A:37:VAL:HG23	1:A:131:THR:HG21	1.85	0.59
1:B:59:GLY:CA	3:B:2006:HOH:O	2.51	0.59
1:C:630:GLN:N	1:C:630:GLN:HE21	2.00	0.59
1:B:231:LEU:HA	1:B:291:ASP:HA	1.84	0.58
1:C:242:ARG:HD3	3:C:2041:HOH:O	2.02	0.58
1:C:450:LYS:HE3	1:C:600:TYR:CZ	2.38	0.58
1:C:546:ASP:OD2	1:C:548:ASP:CB	2.49	0.58
1:A:491:GLN:HA	1:A:494:VAL:HG12	1.83	0.58
1:C:166:ILE:HG12	3:C:2025:HOH:O	2.03	0.58
1:B:388:ASN:CA	3:B:2084:HOH:O	2.50	0.58
1:C:433:ASN:HB3	1:C:434:PRO:HD2	1.85	0.58
1:C:322:PHE:CE2	1:C:324:TYR:HB3	2.39	0.58
1:C:194:ASP:OD1	1:C:195:PHE:N	2.35	0.58
1:A:82:VAL:CG1	1:A:144:ILE:HD11	2.33	0.57
1:C:113:MSE:HG2	1:C:119:LYS:HE2	1.86	0.57
1:B:385:THR:HG22	1:B:385:THR:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:ASP:O	1:C:260:ASP:HB2	2.04	0.57
1:C:118:MSE:HE2	1:C:129:PHE:HB3	1.86	0.57
1:C:275:THR:HG23	3:C:2048:HOH:O	2.03	0.57
1:B:194:ASP:OD1	1:B:195:PHE:N	2.32	0.57
1:C:40:HIS:NE2	1:C:179:HIS:HD2	2.03	0.56
1:C:507:TYR:HA	1:C:510:LEU:HD12	1.87	0.56
1:B:497:LYS:HG2	3:B:2119:HOH:O	2.05	0.56
1:C:411:TYR:HA	1:C:429:TRP:O	2.04	0.56
1:A:256:VAL:HG21	1:A:279:LEU:HD11	1.86	0.56
1:C:141:ILE:HD11	1:C:168:ILE:HD11	1.87	0.56
1:C:507:TYR:HA	1:C:510:LEU:CD1	2.36	0.56
1:A:259:ASP:O	1:A:260:ASP:HB2	2.04	0.56
1:C:240:SER:O	1:C:320:VAL:HA	2.06	0.56
1:A:373:GLN:O	1:A:443:LYS:HD2	2.06	0.56
1:B:564:GLU:OE1	1:B:609:TYR:OH	2.24	0.56
1:A:572:THR:HG21	1:A:592:LYS:HE3	1.87	0.55
1:C:347:LEU:HD11	1:C:426:VAL:HG23	1.88	0.55
1:C:90:ILE:HD12	1:C:100:VAL:HG12	1.87	0.55
1:B:317:SER:HB2	1:B:443:LYS:HD3	1.87	0.55
1:B:162:LYS:O	1:B:163:ALA:HB3	2.05	0.55
1:A:84:THR:CG2	1:A:88:ASN:HA	2.36	0.55
1:A:345:LEU:HD21	1:A:424:ILE:HD12	1.89	0.55
1:A:465:GLU:HG2	1:A:556:VAL:HG22	1.87	0.55
1:B:208:LYS:HD2	1:B:440:THR:OG1	2.07	0.55
1:C:146:SER:HA	1:C:326:ASN:O	2.06	0.55
1:C:573:TYR:HB2	1:C:593:PHE:CZ	2.42	0.55
1:A:162:LYS:NZ	3:A:2027:HOH:O	2.40	0.55
1:A:317:SER:HB2	1:A:443:LYS:HD3	1.88	0.55
1:C:89:GLU:HB2	3:C:2011:HOH:O	2.07	0.55
1:A:629:PRO:C	1:A:630:GLN:HE21	2.09	0.54
1:C:238:ASN:CA	3:C:2039:HOH:O	2.55	0.54
1:B:84:THR:CG2	1:B:85:ASN:O	2.49	0.54
1:B:472:ASP:HB3	1:B:574:TYR:CE2	2.42	0.54
1:A:164:VAL:HG12	3:A:2023:HOH:O	2.07	0.54
1:B:312:VAL:HG12	1:B:313:GLU:HG3	1.88	0.54
1:B:59:GLY:HA2	3:B:2006:HOH:O	2.07	0.54
1:C:548:ASP:HA	3:C:2104:HOH:O	2.07	0.54
1:A:193:LYS:HD3	1:A:441:GLU:HG3	1.90	0.53
1:A:193:LYS:HD2	1:A:320:VAL:CG2	2.38	0.53
1:C:141:ILE:HB	1:C:166:ILE:HD12	1.90	0.53
1:A:113:MSE:HE1	1:A:144:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ILE:CD1	1:C:320:VAL:HG21	2.38	0.53
1:B:347:LEU:O	1:B:389:THR:HA	2.08	0.53
1:B:388:ASN:N	3:B:2084:HOH:O	2.42	0.53
1:C:484:LYS:HG3	1:C:484:LYS:O	2.08	0.53
1:A:164:VAL:CG1	3:A:2023:HOH:O	2.56	0.52
1:C:224:ILE:HD13	1:C:320:VAL:HG11	1.91	0.52
1:C:558:ASP:OD2	1:C:562:ARG:NH2	2.37	0.52
1:B:629:PRO:C	1:B:630:GLN:NE2	2.60	0.52
1:C:206:VAL:O	1:C:206:VAL:HG22	2.08	0.52
1:A:387:LYS:O	1:A:387:LYS:HG3	2.10	0.52
1:B:494:VAL:HG13	1:B:495:THR:N	2.24	0.52
1:A:462:ALA:HB2	1:A:559:ALA:HA	1.92	0.52
1:C:242:ARG:CZ	3:C:2041:HOH:O	2.58	0.52
1:A:481:LYS:HE3	3:A:2137:HOH:O	2.09	0.52
1:A:88:ASN:ND2	1:A:104:PRO:HG3	2.23	0.52
1:B:385:THR:CG2	1:B:385:THR:O	2.58	0.51
1:A:83:TRP:CZ3	1:A:168:ILE:HD11	2.44	0.51
1:C:126:GLY:HA2	3:C:2017:HOH:O	2.10	0.51
1:C:78:GLY:HA2	1:C:121:LEU:HD22	1.93	0.51
1:B:387:LYS:O	1:B:387:LYS:CG	2.57	0.51
1:C:546:ASP:OD1	1:C:548:ASP:HB2	2.11	0.51
1:B:113:MSE:HE1	1:B:144:ILE:HD12	1.92	0.51
1:B:584:TYR:CD2	1:B:625:LYS:HB2	2.46	0.51
1:C:162:LYS:O	1:C:163:ALA:HB3	2.10	0.51
1:C:493:VAL:O	1:C:497:LYS:HB2	2.10	0.51
1:C:228:ILE:HG23	1:C:229:PRO:HD2	1.92	0.50
1:C:482:ALA:O	1:C:485:VAL:HG12	2.11	0.50
1:C:41:LYS:O	1:C:75:GLU:HA	2.12	0.50
1:C:136:ALA:O	1:C:137:ALA:HB2	2.11	0.50
1:B:193:LYS:HD3	1:B:441:GLU:HG3	1.93	0.50
1:C:384:THR:H	1:C:387:LYS:HE3	1.77	0.49
1:B:494:VAL:CG1	1:B:495:THR:N	2.75	0.49
1:C:480:ARG:HA	1:C:540:ALA:O	2.11	0.49
1:C:420:THR:HG22	1:C:421:ALA:N	2.27	0.49
1:B:318:ASN:O	1:B:441:GLU:HG2	2.13	0.49
1:A:72:ASN:OD1	1:A:72:ASN:O	2.31	0.49
1:B:120:LYS:HB2	1:B:129:PHE:CZ	2.47	0.49
1:A:319:ASP:HA	1:A:441:GLU:CD	2.33	0.49
1:A:166:ILE:HD11	1:A:182:PRO:HD3	1.95	0.48
1:A:580:GLN:HG3	1:A:584:TYR:O	2.13	0.48
1:A:603:THR:HG22	1:A:615:LYS:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LEU:HD22	1:C:181:TYR:HB3	1.95	0.48
1:C:500:LEU:HA	1:C:526:ALA:HB1	1.94	0.48
1:C:134:LEU:HB3	1:C:139:TYR:OH	2.14	0.48
1:A:348:THR:HG23	1:A:389:THR:HG22	1.94	0.48
1:B:188:LYS:HG2	1:B:189:PRO:O	2.14	0.48
1:B:335:LYS:HD2	1:B:335:LYS:N	2.28	0.48
1:A:482:ALA:HB2	1:A:551:ASN:HD21	1.79	0.48
1:B:279:LEU:HD23	1:B:279:LEU:C	2.34	0.48
1:A:628:ILE:HA	1:A:629:PRO:HD3	1.66	0.48
1:B:166:ILE:HD11	1:B:182:PRO:HG3	1.95	0.48
1:C:273:VAL:HG12	1:C:274:ALA:N	2.29	0.48
1:C:558:ASP:C	1:C:558:ASP:OD1	2.52	0.48
1:C:342:ASN:N	1:C:342:ASN:ND2	2.60	0.48
1:A:450:LYS:HE2	1:A:600:TYR:O	2.14	0.47
1:A:172:LEU:O	1:A:173:ASN:C	2.52	0.47
1:B:312:VAL:CG1	1:B:313:GLU:HG3	2.43	0.47
1:B:84:THR:HG23	1:B:89:GLU:N	2.28	0.47
1:C:499:ALA:HA	1:C:502:ARG:NH2	2.29	0.47
1:A:89:GLU:HG2	1:A:97:THR:CG2	2.44	0.47
1:C:46:ASP:OD1	1:C:72:ASN:OD1	2.32	0.47
1:A:359:ILE:HB	1:A:360:PRO:HD2	1.96	0.47
1:B:454:VAL:HA	1:B:459:ASN:O	2.14	0.47
1:C:450:LYS:HE3	1:C:600:TYR:CE1	2.49	0.47
1:A:136:ALA:O	1:A:137:ALA:HB2	2.14	0.47
1:B:141:ILE:HD11	1:B:168:ILE:HD11	1.97	0.47
1:C:161:SER:HB3	3:C:2024:HOH:O	2.14	0.47
1:A:41:LYS:HG3	1:A:79:VAL:HG11	1.96	0.47
1:C:240:SER:HB3	1:C:333:THR:HB	1.97	0.47
1:B:145:HIS:HA	3:B:2024:HOH:O	2.14	0.47
1:B:44:ALA:HB2	1:B:52:ILE:CD1	2.45	0.47
1:A:626:ILE:HA	3:A:2169:HOH:O	2.14	0.47
1:B:136:ALA:HA	1:B:170:LEU:O	2.14	0.47
1:B:494:VAL:CG2	3:B:2114:HOH:O	2.61	0.47
1:B:482:ALA:HB2	1:B:551:ASN:ND2	2.30	0.47
1:C:72:ASN:O	1:C:72:ASN:CG	2.53	0.47
1:A:472:ASP:OD1	1:A:473:ASN:N	2.47	0.47
1:B:450:LYS:HE3	1:B:600:TYR:CE2	2.50	0.47
1:B:450:LYS:HE3	1:B:600:TYR:CZ	2.50	0.47
1:C:239:TRP:CZ2	1:C:322:PHE:CE1	3.03	0.47
1:A:162:LYS:HB3	1:A:183:LYS:HB2	1.96	0.46
1:A:322:PHE:HB3	1:A:437:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ASP:OD1	1:A:473:ASN:HB2	2.15	0.46
1:B:347:LEU:HB3	1:B:390:VAL:HG12	1.97	0.46
1:C:52:ILE:HB	1:C:183:LYS:HD3	1.97	0.46
1:A:34:THR:HB	1:A:170:LEU:HD22	1.97	0.46
1:B:447:TYR:CE1	1:B:597:ALA:HA	2.50	0.46
1:B:84:THR:HG23	1:B:88:ASN:C	2.36	0.46
1:A:472:ASP:C	1:A:472:ASP:OD1	2.54	0.46
1:C:420:THR:HG22	1:C:421:ALA:O	2.14	0.46
1:A:331:GLY:HA2	1:A:413:ALA:O	2.15	0.46
1:B:455:ASN:ND2	1:B:459:ASN:HB2	2.30	0.46
1:C:205:ARG:HG2	1:C:207:ASP:OD1	2.16	0.46
1:C:84:THR:CG2	1:C:102:ILE:HD12	2.46	0.46
1:B:282:THR:O	1:B:283:ASP:C	2.54	0.46
1:C:321:THR:HG22	1:C:438:ASP:OD1	2.16	0.46
1:B:256:VAL:HG22	1:B:300:ILE:HG12	1.96	0.46
1:B:61:TYR:CG	1:B:62:ALA:N	2.84	0.46
1:C:75:GLU:HG2	3:C:2017:HOH:O	2.14	0.46
1:A:406:ARG:NH1	3:A:2099:HOH:O	2.38	0.46
1:B:482:ALA:HB2	1:B:551:ASN:HD21	1.80	0.46
1:C:164:VAL:HA	1:C:165:PRO:C	2.35	0.46
1:C:464:ALA:CB	1:C:581:PRO:HD3	2.37	0.46
1:A:337:ASN:OD1	1:A:338:LYS:N	2.46	0.45
1:A:547:LYS:HG2	3:A:2139:HOH:O	2.15	0.45
1:A:85:ASN:C	1:A:85:ASN:OD1	2.55	0.45
1:B:44:ALA:HB2	1:B:52:ILE:HD11	1.97	0.45
1:C:193:LYS:HD3	1:C:441:GLU:HG2	1.98	0.45
1:A:92:ASP:C	1:A:92:ASP:OD1	2.55	0.45
1:B:562:ARG:NH1	1:B:610:THR:OG1	2.44	0.45
1:C:321:THR:CG2	3:C:2088:HOH:O	2.61	0.45
1:C:41:LYS:HD3	1:C:42:LEU:N	2.32	0.45
1:C:233:ASN:O	3:C:2037:HOH:O	2.21	0.45
1:A:383:LEU:HA	1:A:387:LYS:HE3	1.99	0.45
1:A:193:LYS:HD2	1:A:320:VAL:HG21	1.99	0.45
1:C:88:ASN:HB3	1:C:102:ILE:O	2.17	0.45
1:A:525:LYS:HE2	1:A:525:LYS:HB3	1.73	0.45
1:C:176:VAL:HG23	1:C:177:ASP:N	2.32	0.45
1:C:405:GLU:OE2	1:C:413:ALA:HB2	2.17	0.45
1:C:494:VAL:CG1	1:C:495:THR:N	2.80	0.45
1:A:256:VAL:CG2	1:A:279:LEU:HD11	2.47	0.44
1:A:236:THR:OG1	1:A:328:PRO:HA	2.17	0.44
1:A:388:ASN:OD1	1:A:389:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:HA	1:B:104:PRO:HD3	1.84	0.44
1:B:89:GLU:CG	1:B:97:THR:HB	2.46	0.44
1:C:290:ASN:O	1:C:291:ASP:HB2	2.16	0.44
1:B:195:PHE:HB2	1:B:198:LYS:HD3	1.99	0.44
1:B:577:GLU:O	1:B:586:LEU:HD11	2.17	0.44
1:A:630:GLN:N	1:A:630:GLN:HE21	2.15	0.44
1:B:361:ALA:HB3	1:B:385:THR:HG23	2.00	0.44
1:C:358:PRO:O	1:C:359:ILE:HG23	2.17	0.44
1:A:584:TYR:CD2	1:A:625:LYS:HB2	2.52	0.44
1:B:43:LEU:HD23	1:B:44:ALA:C	2.38	0.44
1:C:194:ASP:HA	1:C:442:PRO:HG3	1.99	0.44
1:B:239:TRP:CE2	1:B:322:PHE:CE1	3.06	0.44
1:C:97:THR:HG21	3:C:2013:HOH:O	2.18	0.44
1:A:457:LYS:HB2	1:A:457:LYS:HE3	1.68	0.44
1:B:435:LYS:HB2	1:B:436:PRO:HD2	2.00	0.44
1:C:577:GLU:HG2	1:C:586:LEU:HD12	2.00	0.44
1:C:344:ASP:OD1	1:C:393:ASN:OD1	2.36	0.43
1:C:494:VAL:HG13	1:C:495:THR:N	2.33	0.43
1:A:410:GLY:HA2	1:A:432:GLU:HA	2.01	0.43
1:B:447:TYR:HB3	3:B:2134:HOH:O	2.18	0.43
1:C:476:GLN:HE21	1:C:476:GLN:HB2	1.63	0.43
1:A:87:ASN:O	1:A:88:ASN:HB2	2.18	0.43
1:A:92:ASP:OD2	1:A:96:GLN:HB2	2.17	0.43
1:B:213:ASN:HB2	1:B:447:TYR:CZ	2.53	0.43
1:B:336:PRO:HA	1:B:401:TYR:O	2.18	0.43
1:B:480:ARG:HA	1:B:540:ALA:O	2.19	0.43
1:C:159:THR:HG21	1:C:187:ALA:HB3	2.00	0.43
1:B:157:THR:HG22	1:B:434:PRO:HG2	1.99	0.43
1:A:520:LYS:HG2	1:A:559:ALA:HB1	2.01	0.43
1:C:215:GLN:HB3	1:C:569:LEU:HG	2.01	0.43
1:C:317:SER:HB2	1:C:443:LYS:HD3	2.00	0.43
1:A:138:LYS:HD2	3:A:2007:HOH:O	2.18	0.43
1:A:82:VAL:HG23	1:A:119:LYS:HB3	2.00	0.43
1:B:200:ASN:HA	1:B:201:PRO:HD3	1.89	0.43
1:B:364:GLU:HG2	1:B:384:THR:HA	2.01	0.43
1:C:414:ASP:C	1:C:414:ASP:OD1	2.55	0.43
1:A:205:ARG:HB3	1:A:208:LYS:HG3	2.01	0.42
1:A:498:ASP:O	1:A:501:ASP:HB2	2.19	0.42
1:C:43:LEU:HD21	1:C:186:GLU:HG2	2.01	0.42
1:C:530:TYR:O	1:C:534:VAL:HG23	2.19	0.42
1:A:315:PRO:O	1:A:373:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:VAL:O	1:B:313:GLU:HB2	2.19	0.42
1:C:34:THR:HB	1:C:170:LEU:HD22	2.01	0.42
1:C:456:ASP:OD1	1:C:457:LYS:HG3	2.19	0.42
1:C:629:PRO:C	1:C:630:GLN:NE2	2.66	0.42
1:B:236:THR:CG2	1:B:238:ASN:ND2	2.82	0.42
1:C:40:HIS:NE2	1:C:179:HIS:CD2	2.84	0.42
1:A:215:GLN:O	1:A:306:LEU:HD23	2.19	0.42
1:B:519:GLU:OE1	1:B:522:LYS:HD3	2.20	0.42
1:C:357:ALA:HA	1:C:358:PRO:HD3	1.94	0.42
1:A:193:LYS:HD2	1:A:320:VAL:HG23	2.01	0.42
1:B:320:VAL:HG12	1:B:321:THR:N	2.34	0.42
1:B:44:ALA:CB	1:B:52:ILE:HD11	2.50	0.42
1:A:549:ASN:OD1	1:A:549:ASN:C	2.58	0.42
1:B:459:ASN:N	1:B:459:ASN:HD22	2.18	0.42
1:B:527:GLN:CG	1:B:558:ASP:HB3	2.50	0.42
1:C:472:ASP:OD1	1:C:472:ASP:C	2.58	0.42
1:C:546:ASP:CG	1:C:548:ASP:CB	2.88	0.42
1:A:573:TYR:HB2	1:A:593:PHE:CZ	2.54	0.42
1:B:557:SER:HA	1:B:562:ARG:O	2.19	0.42
1:C:227:LYS:HD2	3:C:2053:HOH:O	2.20	0.42
1:C:273:VAL:HG12	3:C:2048:HOH:O	2.19	0.41
1:B:89:GLU:HG2	1:B:97:THR:HB	2.03	0.41
1:C:388:ASN:O	1:C:389:THR:HG22	2.19	0.41
1:B:519:GLU:OE1	1:B:522:LYS:CD	2.68	0.41
1:B:555:LEU:HD22	1:B:564:GLU:O	2.21	0.41
1:B:239:TRP:CZ2	1:B:322:PHE:CE1	3.09	0.41
1:A:383:LEU:HD11	1:A:390:VAL:HG12	2.02	0.41
1:A:527:GLN:OE1	1:A:527:GLN:C	2.59	0.41
1:A:449:LYS:NZ	1:A:605:GLN:OE1	2.38	0.41
1:C:206:VAL:O	1:C:206:VAL:CG2	2.68	0.41
1:A:273:VAL:HG22	1:A:276:GLY:O	2.19	0.41
1:A:431:ASP:O	1:A:432:GLU:HB2	2.20	0.41
1:A:396:ASP:C	1:A:396:ASP:OD1	2.59	0.41
1:C:83:TRP:CZ2	1:C:141:ILE:HD11	2.56	0.41
1:A:46:ASP:CG	1:A:48:ASP:H	2.23	0.41
1:B:312:VAL:HG23	1:B:566:THR:HB	2.02	0.41
1:A:31:GLY:HA2	1:A:134:LEU:O	2.20	0.41
1:A:170:LEU:HA	1:A:171:PRO:C	2.40	0.41
1:A:480:ARG:HA	1:A:540:ALA:O	2.20	0.41
1:C:466:PHE:CE2	1:C:577:GLU:HB2	2.56	0.41
1:C:90:ILE:HD12	1:C:100:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:PHE:CE2	1:A:324:TYR:HB3	2.56	0.41
1:B:320:VAL:CG1	1:B:321:THR:N	2.84	0.41
1:B:41:LYS:O	1:B:75:GLU:HA	2.21	0.41
1:B:89:GLU:HG2	1:B:97:THR:CG2	2.51	0.41
1:C:254:VAL:HB	3:C:2045:HOH:O	2.21	0.41
1:B:83:TRP:CH2	1:B:168:ILE:CD1	3.03	0.40
1:C:383:LEU:HD12	1:C:390:VAL:HB	2.04	0.40
1:B:228:ILE:HD12	1:B:234:TYR:HE2	1.86	0.40
1:B:240:SER:HB3	1:B:333:THR:HB	2.03	0.40
1:B:378:VAL:O	1:B:379:GLN:CB	2.68	0.40
1:B:384:THR:OG1	1:B:385:THR:N	2.54	0.40
1:C:175:VAL:HA	3:C:2027:HOH:O	2.21	0.40
1:A:176:VAL:HG23	1:A:177:ASP:OD1	2.22	0.40
1:A:519:GLU:O	1:A:522:LYS:HB2	2.22	0.40
1:C:319:ASP:HA	1:C:441:GLU:OE2	2.22	0.40
1:C:497:LYS:HG2	1:C:530:TYR:CE1	2.56	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	602/605 (100%)	566 (94%)	34 (6%)	2 (0%)	43	58
1	B	602/605 (100%)	573 (95%)	25 (4%)	4 (1%)	24	35
1	C	602/605 (100%)	569 (94%)	31 (5%)	2 (0%)	43	58
All	All	1806/1815 (100%)	1708 (95%)	90 (5%)	8 (0%)	36	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	GLY

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Mol	Chain	Res	Type
1	B	61	TYR
1	A	173	ASN
1	B	173	ASN
1	B	379	GLN
1	C	458	ASP
1	B	474	ALA
1	C	71	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/484 (101%)	475 (97%)	14 (3%)	45	66
1	B	489/484 (101%)	481 (98%)	8 (2%)	65	82
1	C	489/484 (101%)	478 (98%)	11 (2%)	55	74
All	All	1467/1452 (101%)	1434 (98%)	33 (2%)	55	74

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	68	VAL
1	A	84	THR
1	A	89	GLU
1	A	105	GLN
1	A	264	GLU
1	A	278	ASP
1	A	373	GLN
1	A	383	LEU
1	A	420	THR
1	A	483	ASP
1	A	490	LYS
1	A	497	LYS
1	A	630	GLN
1	B	60	ASN

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Mol	Chain	Res	Type
1	B	89	GLU
1	B	105	GLN
1	B	264	GLU
1	B	342	ASN
1	B	373	GLN
1	B	497	LYS
1	B	630	GLN
1	C	56	LEU
1	C	60	ASN
1	C	164	VAL
1	C	264	GLU
1	C	342	ASN
1	C	373	GLN
1	C	483	ASP
1	C	510	LEU
1	C	521	GLU
1	C	589	SER
1	C	630	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	94	ASN
1	A	96	GLN
1	A	105	GLN
1	A	179	HIS
1	A	293	ASN
1	A	393	ASN
1	A	491	GLN
1	A	514	GLN
1	A	551	ASN
1	A	630	GLN
1	B	60	ASN
1	B	64	ASN
1	B	101	ASN
1	B	179	HIS
1	B	214	HIS
1	B	293	ASN
1	B	459	ASN
1	B	491	GLN
1	B	630	GLN

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Mol	Chain	Res	Type
1	C	60	ASN
1	C	87	ASN
1	C	179	HIS
1	C	215	GLN
1	C	293	ASN
1	C	342	ASN
1	C	373	GLN
1	C	393	ASN
1	C	459	ASN
1	C	476	GLN
1	C	508	ASN
1	C	531	ASN
1	C	630	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.