



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:02 am BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

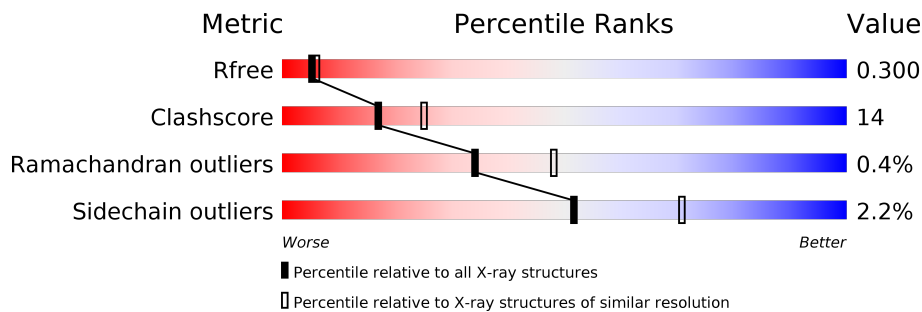
1 Overall quality at a glance

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	605	
1	B	605	
1	C	605	

2 Entry composition [i](#)

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
			Total	C	N	O	Se			
1	A	604	4576	2866	763	942	5	0	0	0
1	B	604	4576	2866	763	942	5	0	0	0
1	C	604	4576	2866	763	942	5	0	0	0

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 3	Ni 3	0	0
2	A	3	Total 3	Ni 3	0	0
2	C	3	Total 3	Ni 3	0	0

- Molecule 3 is water.

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

Continued on next page...

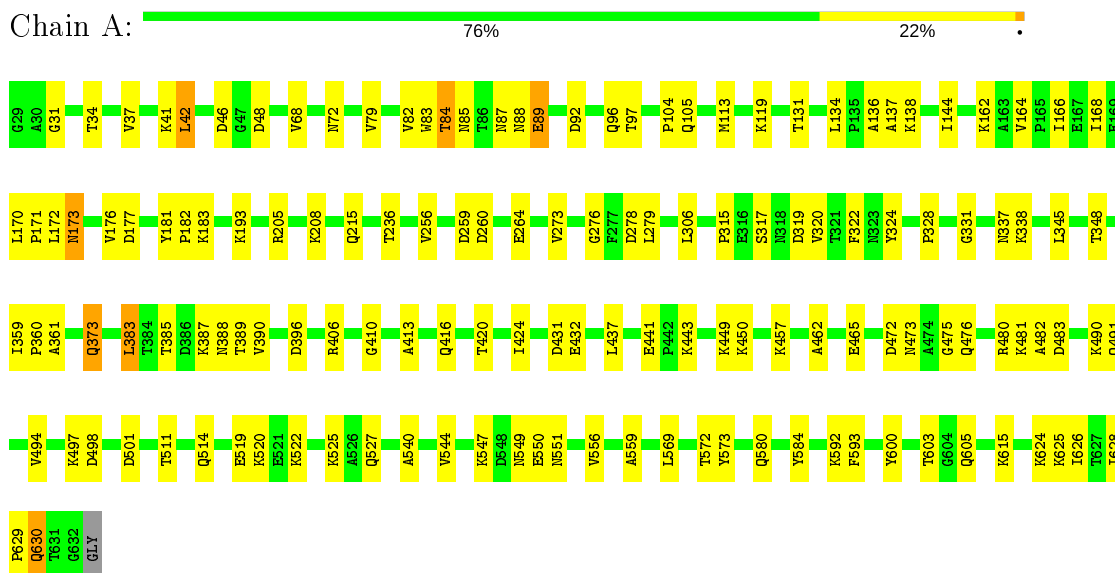
Continued from previous page...

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

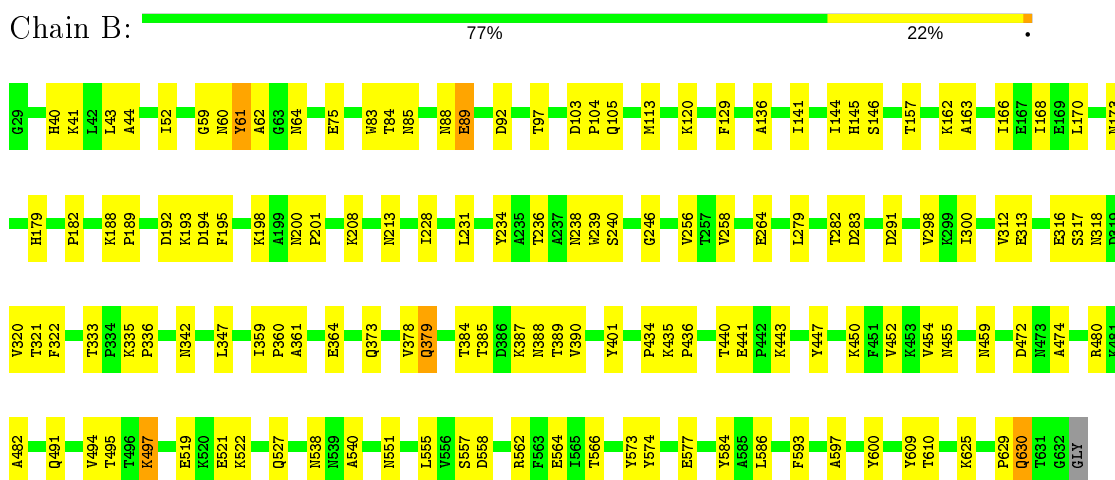
3 Residue-property plots [i](#)

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



- Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



- Molecule 1: CELL WALL SURFACE ANCHOR FAMILY PROTEIN



G29	Y139	V254	E405	V493	T627
T34	K140	D259	G410	V494	I628
H40	I141	D260	Y411	T495	P629
K41	I144	E264	S412	K497	Q630
L42	H145	L270	A413	D498	T631
L43	S146	Y415	D414	A499	G632
D46	T159	V273	Q416	L500	GLY
I52	G160	A274	T420	R502	
L56	S161	T275	A421	Y507	
N60	K162	L279	G422	L510	
Y61	A163	N290	E523	E521	
A62	V164	D291	V426	A526	
P70	E167	T305	W429	Y530	
A71	E168	V312	E432	D546	
N72	E169	E313	N433	R547	
E75	L170	S317	P434	D548	
G78	V175	R318	D438	N549	
V79	V176	D319	E441	A540	
W82	V177	V320	P442	D546	
W83	D177	T321	K443	R547	
T84	A178	F322	K449	V552	
N88	H179	N323	K450	G553	
E89	V180	Y324	F451	K554	
I90	Y181	G325	V452	D558	
T97	P182	N326	D456	A559	
V100	K183	T333	K457	Q560	
M101	E186	N342	D458	G561	
I102	A187	G348	A462	R562	
L109	K193	D344	G463	L569	
M113	D194	L347	A464	Y573	
M118	F195	T348	E465	E577	
K119	R205	A357	F466	P581	
K120	V206	P356	D472	A582	
L121	D207	I359	Q476	G583	
G126	Q215	K376	R480	L586	
F129	I224	L383	K481	S589	
L134	K227	T384	D483	F593	
F135	I228	K367	K484	Y600	
A136	P229	N388	V485	Q605	
A137	N233	T389	E489		
K138	W238	V390	R490		
	S240	N393	I492		
	D241				
	R242				
	A248				

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	41.6	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	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 ²)	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.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	41	55
1	B	602/605 (100%)	573 (95%)	25 (4%)	4 (1%)	22	32
1	C	602/605 (100%)	569 (94%)	31 (5%)	2 (0%)	41	55
All	All	1806/1815 (100%)	1708 (95%)	90 (5%)	8 (0%)	34	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	475	GLY

Continued on next page...

Continued from previous page...

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 [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	489/484 (101%)	475 (97%)	14 (3%)	42	62
1	B	489/484 (101%)	481 (98%)	8 (2%)	62	79
1	C	489/484 (101%)	478 (98%)	11 (2%)	52	71
All	All	1467/1452 (101%)	1434 (98%)	33 (2%)	52	71

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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