



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 03:56 PM EDT

PDB ID : 2QZX  
Title : Secreted aspartic proteinase (Sap) 5 from *Candida albicans*  
Authors : Lee, J.H.; Ruge, E.; Borelli, C.; Maskos, K.; Huber, R.  
Deposited on : 2007-08-17  
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

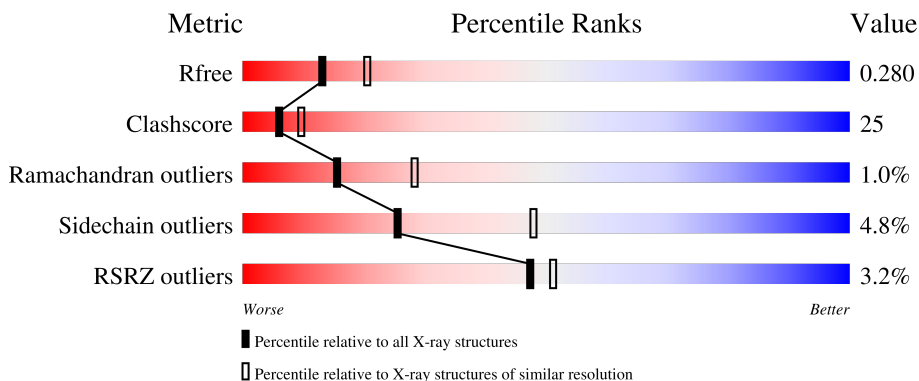
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	342	 3% 60% 37%
1	B	342	 3% 59% 38%
2	C	6	 67% 17% 17%
2	D	6	 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STA	D	2006	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5712 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 Candidapepsin-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2623	1655	443	519	6	0	0	0
1	B	342	2623	1655	443	519	6	0	0	0

- Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	6	48	34	5	9	0	0	0
2	D	6	48	34	5	9	0	0	0

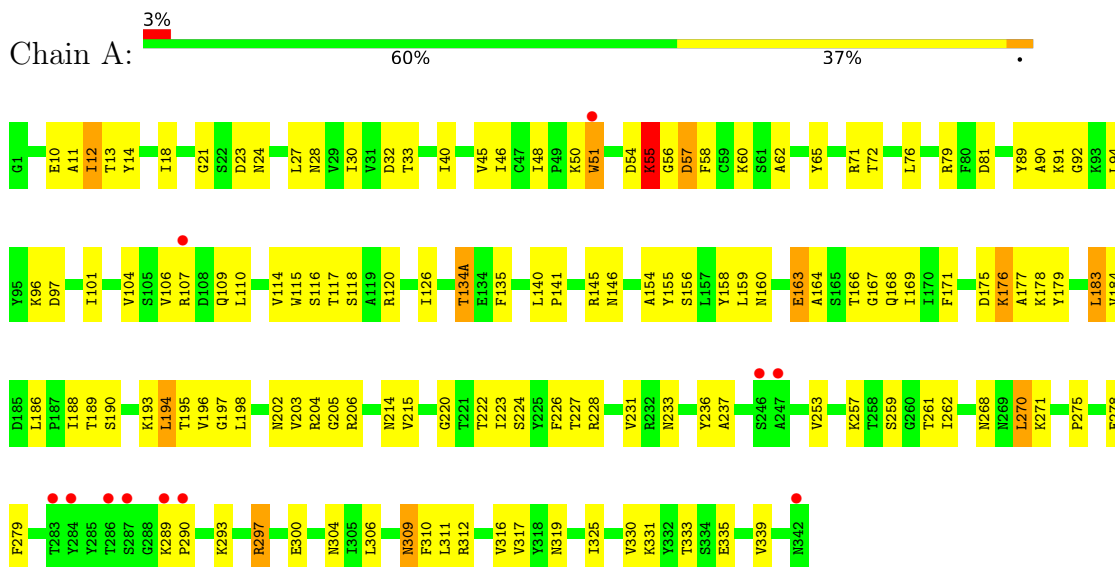
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total 198	O 198	1	0
3	B	169	Total 169	O 169	0	0
3	C	3	Total 3	O 3	0	0

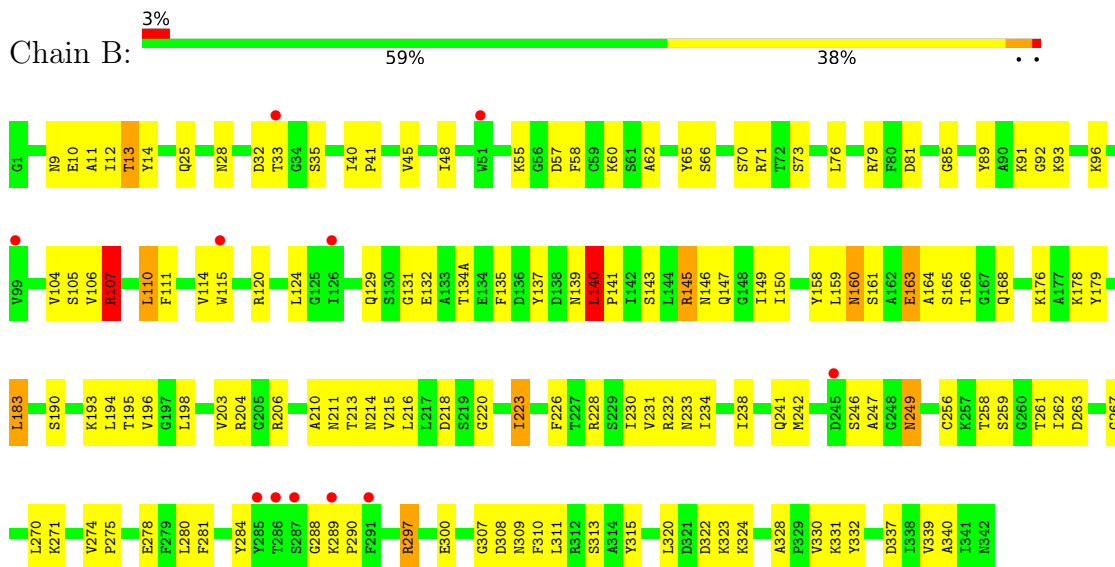
### 3 Residue-property plots [i](#)

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

- Molecule 1: Candidapepsin-5

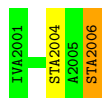


- Molecule 1: Candidapepsin-5



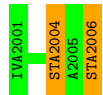
- Molecule 2: Pepstatin

Chain C:  67% 17% 17%



● Molecule 2: Pepstatin

Chain D:  67% 33%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.20Å 92.20Å 182.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.15 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.50) 99.8 (29.15-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.86 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.275 0.224 , 0.280	Depositor DCC
$R_{free}$ test set	1351 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5742e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: IVA, STA

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	0.38	0/2670	0.63	0/3615
1	B	0.39	0/2670	0.66	3/3615 (0.1%)
2	C	0.38	0/17	1.16	0/21
2	D	0.38	0/17	0.88	0/21
All	All	0.38	0/5374	0.65	3/7272 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	140	LEU	CA-CB-CG	5.28	127.44	115.30
1	B	110	LEU	CA-CB-CG	5.22	127.31	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	2004	STA	Peptide,Mainchain

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Mol	Chain	Res	Type	Group
2	D	2004	STA	Peptide,Mainchain

## 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	2623	0	2599	130	0
1	B	2623	0	2599	133	0
2	C	48	0	60	3	0
2	D	48	0	60	8	0
3	A	198	0	0	7	0
3	B	169	0	0	17	0
3	C	3	0	0	0	0
All	All	5712	0	5318	264	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 25.

All (264) 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:339:VAL:HB	3:B:3099:HOH:O	1.59	1.02
1:B:258:THR:HB	3:B:3092:HOH:O	1.59	1.02
1:A:11:ALA:O	1:A:12:ILE:HD12	1.63	0.98
1:B:195:THR:HG21	1:B:214:ASN:HB3	1.45	0.96
1:B:25:GLN:HE22	1:B:66:SER:H	1.08	0.93
1:A:134(A):THR:HG22	1:A:135:PHE:H	1.32	0.91
1:A:55:LYS:H	1:A:55:LYS:HD3	1.39	0.88
1:A:106:VAL:HG11	1:A:109:GLN:HE21	1.38	0.88
1:B:129:GLN:O	1:B:132:GLU:HG3	1.73	0.87
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.37	0.87
1:A:253:VAL:CG1	1:A:293:LYS:HB2	2.05	0.86
1:A:195:THR:HG21	1:A:214:ASN:HB3	1.60	0.81
1:B:195:THR:CG2	1:B:214:ASN:HB3	2.10	0.81
1:A:28:ASN:HB3	1:A:62:ALA:HB1	1.63	0.80
1:B:115:TRP:HB3	3:B:3061:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:HB2	1:B:14:TYR:CE2	2.17	0.79
1:A:275:PRO:HB3	1:B:275:PRO:HB3	1.64	0.78
1:A:101:ILE:HD13	1:A:140:LEU:HD21	1.63	0.78
1:B:176:LYS:HE2	3:B:3099:HOH:O	1.85	0.77
1:B:149:ILE:HG22	1:B:150:ILE:HG23	1.65	0.77
1:B:57:ASP:HB3	1:B:60:LYS:HG2	1.67	0.77
1:B:25:GLN:NE2	1:B:66:SER:H	1.83	0.76
1:A:290:PRO:HG2	1:B:284:TYR:CE2	2.22	0.75
1:A:18:ILE:HG22	1:A:101:ILE:HG22	1.70	0.73
1:A:72:THR:HG23	1:A:97:ASP:OD1	1.88	0.72
1:B:48:ILE:HD12	1:B:89:TYR:OH	1.90	0.72
1:B:206:ARG:HE	1:B:233:ASN:HD22	1.37	0.72
1:A:195:THR:CG2	1:A:214:ASN:HB3	2.20	0.72
1:B:81:ASP:OD1	1:B:91:LYS:HG2	1.89	0.72
1:B:107:ARG:HH11	1:B:107:ARG:CG	2.02	0.72
2:D:2006:STA:OXT	2:D:2006:STA:HA	1.87	0.71
1:B:176:LYS:HE3	1:B:337:ASP:OD2	1.91	0.71
1:B:25:GLN:HE22	1:B:66:SER:N	1.87	0.71
1:A:231:VAL:HG11	1:A:300:GLU:HB3	1.74	0.69
1:A:12:ILE:HG23	1:A:222:THR:OG1	1.92	0.69
1:B:281:PHE:HB2	1:B:297:ARG:HD2	1.74	0.69
1:A:72:THR:HG21	3:A:2014:HOH:O	1.93	0.68
1:B:258:THR:CG2	1:B:280:LEU:HD11	2.22	0.68
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.59	0.67
1:B:57:ASP:CB	1:B:60:LYS:HG2	2.25	0.66
1:B:160:ASN:HB3	1:B:164:ALA:HB3	1.76	0.66
1:A:163:GLU:CG	1:B:258:THR:HA	2.25	0.66
1:A:57:ASP:HB2	1:A:60:LYS:HG2	1.78	0.66
1:B:76:LEU:HD11	1:B:96:LYS:HG3	1.79	0.65
1:B:258:THR:HG22	1:B:280:LEU:HD11	1.77	0.65
1:A:14:TYR:OH	1:A:312:ARG:HD3	1.94	0.65
1:A:333:THR:HG22	1:A:335:GLU:H	1.61	0.65
1:B:297:ARG:HD3	3:B:3043:HOH:O	1.95	0.65
1:A:215:VAL:HG12	1:A:304:ASN:HB3	1.79	0.64
1:B:139:ASN:HB2	3:B:3097:HOH:O	1.97	0.64
1:A:223:ILE:CG2	1:A:297:ARG:HG3	2.29	0.63
1:B:203:VAL:HG22	1:B:262:ILE:HG23	1.80	0.63
1:A:179:TYR:CE2	1:A:183:LEU:HD13	2.33	0.63
1:A:186:LEU:HD13	1:A:196:VAL:HG11	1.80	0.63
1:A:206:ARG:HD2	1:A:237:ALA:HB2	1.80	0.62
1:B:28:ASN:HB3	1:B:62:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASP:OD1	1:B:220:GLY:HA3	1.99	0.62
1:B:198:LEU:HD22	1:B:215:VAL:HG11	1.80	0.62
1:B:232:ARG:HB2	3:B:3088:HOH:O	1.98	0.62
1:B:107:ARG:HG2	1:B:147:GLN:OE1	1.99	0.62
1:A:203:VAL:HG12	1:A:204:ARG:HG3	1.82	0.62
1:B:194:LEU:HD21	1:B:320:LEU:HD22	1.82	0.62
1:A:198:LEU:HD22	1:A:215:VAL:HG11	1.81	0.62
1:A:253:VAL:HG13	1:A:293:LYS:HB2	1.80	0.61
1:A:55:LYS:H	1:A:55:LYS:CD	2.10	0.61
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.65	0.61
1:B:40:ILE:HD12	1:B:65:TYR:HB2	1.83	0.61
1:B:206:ARG:HE	1:B:233:ASN:ND2	1.98	0.61
1:B:13:THR:HG23	1:B:14:TYR:N	2.16	0.61
1:B:145:ARG:HG3	1:B:146:ASN:N	2.16	0.61
1:B:106:VAL:HG23	1:B:147:GLN:NE2	2.16	0.60
1:B:33:THR:OG1	1:B:218:ASP:HA	2.02	0.60
1:A:145:ARG:HH21	1:A:146:ASN:HD21	1.50	0.59
1:B:247:ALA:HB3	1:B:249:ASN:OD1	2.02	0.59
2:D:2006:STA:N	2:D:2006:STA:CD1	2.64	0.59
1:B:179:TYR:CE2	1:B:183:LEU:HD13	2.37	0.59
1:A:48:ILE:HD11	1:A:89:TYR:HE2	1.68	0.58
1:A:79:ARG:HG3	3:A:2166:HOH:O	2.04	0.58
1:B:93:LYS:HE2	3:B:3061:HOH:O	2.02	0.58
1:B:158:TYR:CE1	1:B:178:LYS:HD2	2.39	0.58
1:B:210:ALA:HB1	1:B:213:THR:HG22	1.86	0.58
1:B:79:ARG:HG3	1:B:79:ARG:HH11	1.69	0.57
1:A:50:LYS:HZ2	1:A:51:TRP:HZ3	1.51	0.57
1:A:206:ARG:HE	1:A:236:TYR:HD2	1.53	0.57
1:A:163:GLU:HG3	1:B:258:THR:HA	1.84	0.57
1:A:176:LYS:HE3	1:A:339:VAL:HG21	1.86	0.57
1:A:18:ILE:HG22	1:A:101:ILE:CG2	2.33	0.56
1:B:226:PHE:HB2	1:B:231:VAL:CG2	2.35	0.56
1:B:106:VAL:HG21	1:B:143:SER:HB3	1.87	0.56
1:A:163:GLU:HG2	1:B:258:THR:HA	1.88	0.56
1:B:168:GLN:NE2	3:B:3148:HOH:O	2.39	0.56
2:D:2006:STA:HD12	2:D:2006:STA:OH	2.06	0.56
1:A:184:VAL:HG13	1:A:268:ASN:ND2	2.21	0.56
1:A:228:ARG:O	1:A:231:VAL:HG12	2.06	0.56
1:A:231:VAL:HG11	1:A:300:GLU:CB	2.37	0.55
1:A:167:GLY:O	1:A:168:GLN:HG2	2.07	0.55
1:B:140:LEU:HD12	1:B:141:PRO:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HE2	3:B:3165:HOH:O	2.07	0.55
1:B:124:LEU:HD21	1:B:140:LEU:HD21	1.88	0.55
2:D:2006:STA:HD12	2:D:2006:STA:CH	2.36	0.55
1:A:309:ASN:HD22	1:A:310:PHE:N	2.05	0.54
1:A:54:ASP:HB3	1:A:58:PHE:CD2	2.42	0.54
1:B:85:GLY:HA2	2:D:2006:STA:HD22	1.88	0.54
1:B:160:ASN:HB3	1:B:164:ALA:CB	2.37	0.54
1:B:267:GLY:HA2	3:B:3053:HOH:O	2.08	0.54
1:A:134(A):THR:HG22	1:A:135:PHE:O	2.08	0.54
2:C:2006:STA:OH	2:C:2006:STA:HD22	2.08	0.54
1:B:60:LYS:HD3	3:B:3089:HOH:O	2.08	0.53
1:A:40:ILE:HD12	1:A:65:TYR:HB2	1.90	0.53
1:A:126:ILE:HD12	1:A:155:TYR:CZ	2.43	0.53
1:B:258:THR:HG22	1:B:280:LEU:CD1	2.37	0.53
1:A:134(A):THR:HG23	1:A:135:PHE:CD1	2.44	0.53
1:B:10:GLU:O	1:B:11:ALA:HB3	2.08	0.53
1:B:161:SER:HB3	1:B:332:TYR:CZ	2.44	0.53
1:B:275:PRO:HG2	1:B:278:GLU:HG2	1.91	0.53
1:A:12:ILE:O	1:A:12:ILE:CG2	2.57	0.52
1:A:134(A):THR:HG22	1:A:135:PHE:N	2.14	0.52
1:B:93:LYS:NZ	3:B:3105:HOH:O	2.40	0.52
1:A:11:ALA:C	1:A:12:ILE:HD12	2.30	0.52
2:C:2006:STA:N	2:C:2006:STA:CD2	2.73	0.52
1:A:262:ILE:HD12	1:A:279:PHE:CD1	2.44	0.52
1:B:140:LEU:HD12	1:B:141:PRO:CD	2.40	0.52
1:A:289:LYS:NZ	3:A:2159:HOH:O	2.42	0.51
1:B:134(A):THR:HG23	1:B:135:PHE:H	1.74	0.51
1:A:12:ILE:HG13	1:A:222:THR:HG21	1.92	0.51
1:A:189:THR:OG1	1:A:195:THR:HG22	2.10	0.51
1:A:106:VAL:HG12	1:A:109:GLN:HB2	1.93	0.51
1:A:101:ILE:CD1	1:A:140:LEU:HD21	2.37	0.50
1:B:13:THR:O	1:B:14:TYR:CD1	2.64	0.50
1:A:155:TYR:HB3	1:A:171:PHE:HA	1.94	0.50
1:A:179:TYR:CD2	1:A:183:LEU:HD13	2.47	0.50
1:A:120:ARG:HG2	1:A:120:ARG:NH1	2.25	0.50
1:A:134(A):THR:HG23	1:A:135:PHE:CE1	2.46	0.49
1:B:163:GLU:H	1:B:163:GLU:CD	2.15	0.49
1:A:48:ILE:HD11	1:A:89:TYR:CE2	2.46	0.49
1:B:158:TYR:CZ	1:B:178:LYS:HD2	2.48	0.49
1:A:176:LYS:HA	1:A:179:TYR:CE1	2.47	0.49
1:B:183:LEU:HD12	1:B:328:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ARG:HD2	1:B:259:SER:O	2.13	0.49
1:A:92:GLY:HA3	1:A:114:VAL:HA	1.94	0.49
1:A:106:VAL:HG11	1:A:109:GLN:NE2	2.19	0.49
1:A:290:PRO:HG2	1:B:284:TYR:HE2	1.74	0.49
1:B:323:LYS:HD2	3:B:3065:HOH:O	2.12	0.49
1:A:76:LEU:HD11	1:A:96:LYS:HG3	1.94	0.49
1:B:158:TYR:HB2	1:B:315:TYR:CE1	2.48	0.49
1:B:190:SER:HB3	1:B:193:LYS:O	2.12	0.48
1:B:168:GLN:HG2	3:B:3124:HOH:O	2.12	0.48
1:B:258:THR:HG23	1:B:258:THR:O	2.13	0.48
1:A:107:ARG:HG2	1:A:107:ARG:HH11	1.78	0.48
1:A:12:ILE:HG23	1:A:222:THR:HG1	1.78	0.48
1:A:270:LEU:HD22	1:A:271:LYS:N	2.28	0.48
1:B:161:SER:HB3	1:B:332:TYR:CE2	2.48	0.48
1:B:226:PHE:HB2	1:B:231:VAL:HG23	1.95	0.48
1:A:159:LEU:HB3	1:A:312:ARG:HG2	1.94	0.48
1:A:293:LYS:HE2	3:A:2114:HOH:O	2.14	0.48
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.27	0.48
1:B:289:LYS:HG3	1:B:290:PRO:HD2	1.95	0.48
1:B:32:ASP:OD2	1:B:35:SER:HB2	2.15	0.47
1:A:115:TRP:CE3	1:A:116:SER:HB2	2.49	0.47
1:B:93:LYS:HD2	1:B:93:LYS:N	2.29	0.47
1:B:228:ARG:HB3	1:B:300:GLU:CD	2.34	0.47
1:A:140:LEU:HB3	1:A:141:PRO:HD3	1.97	0.47
1:B:263:ASP:HB3	1:B:271:LYS:HE3	1.95	0.47
1:A:134(A):THR:CG2	1:A:135:PHE:H	2.16	0.47
1:A:94:LEU:HD22	1:A:110:LEU:HD21	1.97	0.47
1:A:156:SER:OG	1:A:317:VAL:HG22	2.14	0.47
1:A:297:ARG:HG2	3:A:2153:HOH:O	2.14	0.47
1:B:106:VAL:CG2	1:B:143:SER:HB3	2.45	0.47
1:B:124:LEU:HD11	1:B:140:LEU:HG	1.97	0.47
1:A:32:ASP:OD1	1:A:220:GLY:HA3	2.14	0.47
1:A:48:ILE:HD11	1:A:118:SER:HB3	1.96	0.47
1:A:55:LYS:HD3	1:A:55:LYS:N	2.20	0.46
1:A:91:LYS:O	1:A:114:VAL:HG13	2.16	0.46
1:B:218:ASP:OD2	2:D:2004:STA:OH	2.31	0.46
1:A:275:PRO:HG2	1:A:278:GLU:HG2	1.96	0.46
1:B:195:THR:HG22	1:B:196:VAL:N	2.30	0.46
1:A:48:ILE:O	1:A:48:ILE:HG13	2.15	0.46
1:A:330:VAL:HG22	1:A:331:LYS:N	2.31	0.46
1:B:79:ARG:HG3	1:B:79:ARG:NH1	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:GLN:HB3	3:B:3033:HOH:O	2.14	0.46
1:A:259:SER:HB2	1:B:161:SER:HB2	1.98	0.46
1:B:159:LEU:HD12	1:B:311:LEU:HB2	1.96	0.46
1:B:308:ASP:C	1:B:310:PHE:H	2.20	0.46
2:C:2006:STA:N	2:C:2006:STA:HD23	2.30	0.46
1:A:179:TYR:CZ	1:A:183:LEU:HD13	2.50	0.46
1:A:202:ASN:HA	1:A:206:ARG:O	2.16	0.46
1:B:106:VAL:HG23	1:B:147:GLN:HE22	1.81	0.46
1:B:41:PRO:HB2	1:B:45:VAL:HG11	1.98	0.45
1:B:203:VAL:HG12	1:B:204:ARG:HG3	1.98	0.45
1:A:27:LEU:HD22	1:A:40:ILE:HB	1.98	0.45
1:A:223:ILE:HG13	1:A:224:SER:N	2.30	0.45
1:A:290:PRO:HD3	1:B:288:GLY:O	2.16	0.45
1:B:13:THR:HG21	3:B:3006:HOH:O	2.15	0.45
1:A:311:LEU:HD22	1:A:316:VAL:HG21	1.98	0.45
1:B:213:THR:OG1	1:B:214:ASN:N	2.49	0.45
1:B:241:GLN:HG2	1:B:242:MET:N	2.32	0.45
1:A:114:VAL:HG11	1:A:117:THR:HB	1.99	0.45
1:A:13:THR:OG1	1:A:30:ILE:HG23	2.17	0.44
1:B:183:LEU:HD12	1:B:328:ALA:HB2	1.98	0.44
1:B:322:ASP:O	1:B:324:LYS:HG3	2.18	0.44
1:B:330:VAL:HG22	1:B:331:LYS:N	2.32	0.44
1:B:210:ALA:O	1:B:211:ASN:C	2.56	0.44
1:A:54:ASP:HB3	1:A:58:PHE:CE2	2.53	0.44
1:A:55:LYS:HE2	1:A:58:PHE:CB	2.47	0.43
1:A:154:ALA:CB	1:A:319:ASN:HA	2.47	0.43
1:A:331:LYS:HD2	3:A:2120:HOH:O	2.16	0.43
1:B:65:TYR:CE2	1:B:111:PHE:HZ	2.36	0.43
1:B:107:ARG:HG3	1:B:107:ARG:NH1	2.16	0.43
1:B:195:THR:HG23	1:B:215:VAL:C	2.38	0.43
1:A:45:VAL:HG22	1:A:46:ILE:N	2.34	0.43
1:A:195:THR:CG2	1:A:196:VAL:N	2.82	0.43
1:A:81:ASP:OD1	1:A:91:LYS:HG2	2.18	0.43
1:A:190:SER:HB3	1:A:193:LYS:O	2.18	0.43
1:B:65:TYR:CZ	1:B:111:PHE:HZ	2.36	0.43
1:A:57:ASP:HB2	1:A:60:LYS:CG	2.46	0.43
1:B:32:ASP:OD2	1:B:35:SER:CB	2.66	0.43
1:A:160:ASN:HB3	1:A:164:ALA:CB	2.49	0.43
1:A:196:VAL:CG1	1:A:197:GLY:N	2.82	0.43
1:A:204:ARG:NE	1:A:259:SER:O	2.46	0.43
1:A:253:VAL:HG11	1:A:293:LYS:HB2	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134(A):THR:HG21	1:B:137:TYR:HD1	1.83	0.43
1:A:90:ALA:HB1	1:A:114:VAL:HG21	2.01	0.43
1:B:165:SER:OG	1:B:166:THR:HG23	2.19	0.43
1:A:107:ARG:HG2	1:A:107:ARG:NH1	2.34	0.42
1:A:156:SER:O	1:A:169:ILE:HA	2.19	0.42
1:A:175:ASP:O	1:A:177:ALA:N	2.51	0.42
1:A:206:ARG:NH1	1:A:233:ASN:OD1	2.53	0.42
1:B:194:LEU:O	1:B:216:LEU:HD12	2.19	0.42
1:A:186:LEU:HD13	1:A:196:VAL:CG1	2.47	0.42
1:A:188:ILE:CG1	1:A:325:ILE:HG13	2.49	0.42
1:A:279:PHE:O	1:A:297:ARG:HB2	2.19	0.42
1:A:10:GLU:O	1:A:11:ALA:HB3	2.20	0.42
1:A:158:TYR:CE1	1:A:178:LYS:HD3	2.55	0.42
1:B:223:ILE:O	1:B:307:GLY:HA3	2.20	0.42
1:B:226:PHE:HB2	1:B:231:VAL:HG22	2.00	0.42
1:B:261:THR:HG23	1:B:263:ASP:OD1	2.19	0.42
1:A:23:ASP:OD1	1:A:23:ASP:N	2.51	0.42
1:B:104:VAL:CG1	1:B:105:SER:N	2.82	0.42
1:B:238:ILE:O	1:B:238:ILE:HG22	2.20	0.42
1:B:58:PHE:CE1	1:B:120:ARG:NH2	2.88	0.42
1:B:106:VAL:O	1:B:106:VAL:HG13	2.19	0.42
1:B:145:ARG:HA	1:B:150:ILE:O	2.19	0.42
1:B:234:ILE:O	1:B:238:ILE:HG13	2.19	0.42
1:B:70:SER:HB3	1:B:73:SER:HB3	2.02	0.41
1:B:129:GLN:C	1:B:131:GLY:H	2.22	0.41
1:A:158:TYR:CZ	1:A:178:LYS:HD3	2.55	0.41
1:B:226:PHE:O	1:B:231:VAL:CG2	2.69	0.41
1:A:21:GLY:HA2	1:A:97:ASP:OD1	2.20	0.41
1:A:184:VAL:CG1	1:A:268:ASN:ND2	2.83	0.41
1:B:274:VAL:HG13	1:B:313:SER:OG	2.20	0.41
1:A:71:ARG:O	1:A:71:ARG:HG2	2.20	0.41
1:A:226:PHE:HZ	1:A:306:LEU:HD21	1.86	0.41
1:B:92:GLY:HA2	1:B:115:TRP:HD1	1.86	0.41
1:A:309:ASN:HD22	1:A:309:ASN:N	2.17	0.41
2:D:2006:STA:N	2:D:2006:STA:HD13	2.34	0.41
2:D:2006:STA:N	2:D:2006:STA:HD12	2.34	0.40
1:A:160:ASN:HB2	1:A:166:THR:O	2.22	0.40
1:A:24:ASN:ND2	3:A:2030:HOH:O	2.53	0.40
1:A:202:ASN:HD21	1:A:205:GLY:HA2	1.87	0.40
1:B:9:ASN:HB2	1:B:14:TYR:HE2	1.80	0.40
1:B:92:GLY:HA3	1:B:114:VAL:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLY:C	1:B:93:LYS:HD2	2.42	0.40
1:A:33:THR:HB	1:A:194:LEU:HD23	2.03	0.40
1:B:339:VAL:HG22	1:B:340:ALA:N	2.36	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	340/342 (99%)	320 (94%)	16 (5%)	4 (1%)	13	24
1	B	340/342 (99%)	313 (92%)	24 (7%)	3 (1%)	17	31
2	C	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	D	3/6 (50%)	3 (100%)	0	0	100	100
All	All	686/696 (99%)	638 (93%)	41 (6%)	7 (1%)	15	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	56	GLY
1	A	176	LYS
1	B	160	ASN
1	B	12	ILE
1	B	223	ILE
1	A	12	ILE

### 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	289/289 (100%)	276 (96%)	13 (4%)	27	51
1	B	289/289 (100%)	274 (95%)	15 (5%)	23	44
2	C	2/2 (100%)	2 (100%)	0	100	100
2	D	2/2 (100%)	2 (100%)	0	100	100
All	All	582/582 (100%)	554 (95%)	28 (5%)	25	48

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TRP
1	A	55	LYS
1	A	57	ASP
1	A	104	VAL
1	A	134(A)	THR
1	A	163	GLU
1	A	183	LEU
1	A	194	LEU
1	A	227	THR
1	A	261	THR
1	A	270	LEU
1	A	297	ARG
1	A	309	ASN
1	B	13	THR
1	B	55	LYS
1	B	107	ARG
1	B	110	LEU
1	B	140	LEU
1	B	145	ARG
1	B	163	GLU
1	B	183	LEU
1	B	230	ILE
1	B	246	SER
1	B	249	ASN
1	B	256	CYS
1	B	270	LEU
1	B	297	ARG
1	B	309	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	44	ASN
1	A	109	GLN
1	A	113	ASN
1	A	146	ASN
1	A	202	ASN
1	A	211	ASN
1	A	214	ASN
1	A	249	ASN
1	A	268	ASN
1	A	309	ASN
1	B	24	ASN
1	B	25	GLN
1	B	74	GLN
1	B	233	ASN
1	B	309	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	STA	D	2004	2	10,10,11	0.52	0	9,12,14	0.79	0
2	STA	C	2004	2	10,10,11	0.55	0	9,12,14	0.85	0
2	STA	C	2006	2	11,11,11	0.67	0	11,14,14	1.14	1 (9%)
2	STA	D	2006	2	11,11,11	0.63	0	11,14,14	1.64	3 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	STA	D	2004	2	-	2/11/11/12	-
2	STA	C	2004	2	-	1/11/11/12	-
2	STA	C	2006	2	-	5/12/12/12	-
2	STA	D	2006	2	-	9/12/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2006	STA	CM-CH-CA	-3.58	107.32	112.94
2	D	2006	STA	CH-CM-C	-2.64	108.22	114.03
2	C	2006	STA	CM-CH-CA	-2.57	108.91	112.94
2	D	2006	STA	CG-CB-CA	-2.16	111.18	115.82

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2004	STA	O-C-CM-CH
2	D	2004	STA	N-CA-CB-CG
2	D	2004	STA	O-C-CM-CH
2	C	2006	STA	CB-CA-CH-OH
2	D	2006	STA	N-CA-CH-OH
2	D	2006	STA	N-CA-CH-CM
2	D	2006	STA	CB-CA-CH-OH
2	D	2006	STA	CB-CA-CH-CM
2	D	2006	STA	CA-CH-CM-C
2	C	2006	STA	CA-CB-CG-CD1
2	C	2006	STA	CA-CB-CG-CD2
2	D	2006	STA	CA-CB-CG-CD1
2	C	2006	STA	CA-CH-CM-C
2	C	2006	STA	CB-CA-CH-CM
2	D	2006	STA	OXT-C-CM-CH
2	D	2006	STA	CH-CA-CB-CG
2	D	2006	STA	OH-CH-CM-C

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2004	STA	1	0
2	C	2006	STA	3	0
2	D	2006	STA	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	342/342 (100%)	-0.04	11 (3%) 47 51	7, 21, 45, 79	0
1	B	342/342 (100%)	0.06	11 (3%) 47 51	10, 24, 52, 74	0
2	C	3/6 (50%)	0.51	0 100 100	10, 10, 16, 30	0
2	D	3/6 (50%)	-0.29	0 100 100	11, 11, 12, 27	0
All	All	690/696 (99%)	0.01	22 (3%) 47 51	7, 23, 51, 79	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	THR	4.5
1	B	291	PHE	4.4
1	A	287	SER	3.9
1	A	284	TYR	3.4
1	A	51	TRP	3.4
1	B	289	LYS	3.1
1	B	245	ASP	3.0
1	B	286	THR	2.9
1	B	115	TRP	2.8
1	B	51	TRP	2.7
1	A	290	PRO	2.6
1	A	246	SER	2.6
1	B	287	SER	2.4
1	B	126	ILE	2.3
1	A	247	ALA	2.2
1	A	342	ASN	2.2
1	B	33	THR	2.1
1	A	107	ARG	2.1
1	A	289	LYS	2.1
1	B	285	TYR	2.1
1	B	99	VAL	2.1
1	A	283	THR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	STA	C	2006	12/12	0.89	0.19	35,40,44,49	0
2	STA	D	2006	12/12	0.89	0.22	39,51,59,60	0
2	STA	C	2004	11/12	0.94	0.16	10,16,27,32	0
2	STA	D	2004	11/12	0.94	0.17	8,15,18,19	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.