WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Mar 15, 2017 – 05:02 PM EDT

PDB ID	:	5U95
Title	:	Structure of the open conformation of 4-coumarate-CoA ligase from Nicotiana tabacum
Authors	:	Morioka, W.P.; Bianchetti, C.M.
Deposited on	:	2016-12-15
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

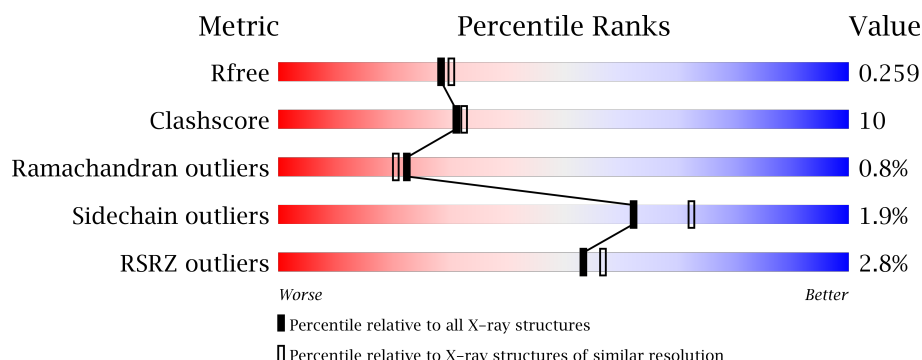|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		10
Ramachandran outliers		0.8%
Sidechain outliers		1.9%
RSRZ outliers		2.8%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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. 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 <=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	542	65% 13% 22%
1	B	542	3% 73% 22% · ·
1	C	542	4% 75% 20% · ·
1	D	542	3% 72% 19% · 7%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	A	601	-	-	-	X
2	CA	A	602	-	-	-	X
2	CA	D	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15622 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 4-coumarate–CoA ligase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3260	2090	534	615	21			
1	B	527	Total	C	N	O	S	0	0	0
			4055	2605	670	758	22			
1	C	522	Total	C	N	O	S	0	1	0
			4028	2589	665	752	22			
1	D	502	Total	C	N	O	S	0	0	0
			3869	2490	633	724	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	272	SER	ARG	conflict	UNP O24146
B	272	SER	ARG	conflict	UNP O24146
C	272	SER	ARG	conflict	UNP O24146
D	272	SER	ARG	conflict	UNP O24146

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

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	2	Total	Ca	0	0
			2	2		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total 129	O 129	0	0
3	B	69	Total 69	O 69	0	0
3	C	81	Total 81	O 81	0	0
3	D	126	Total 126	O 126	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 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.
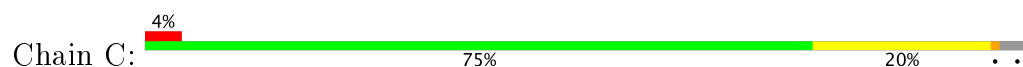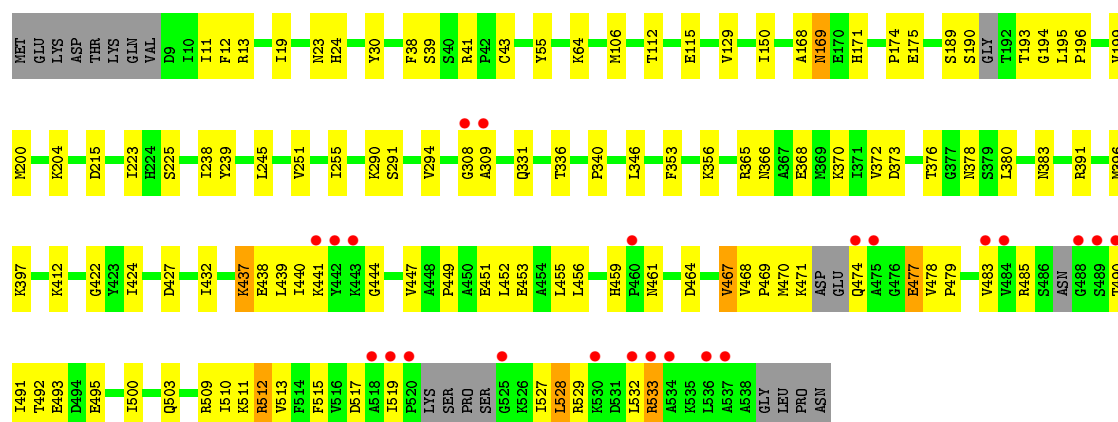
- Molecule 1: 4-coumarate–CoA ligase 2
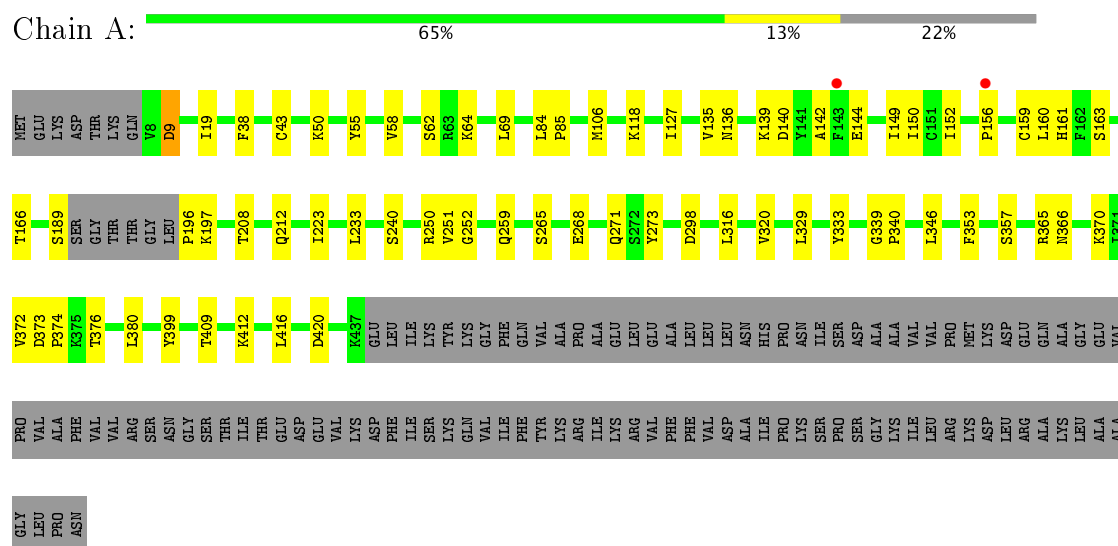
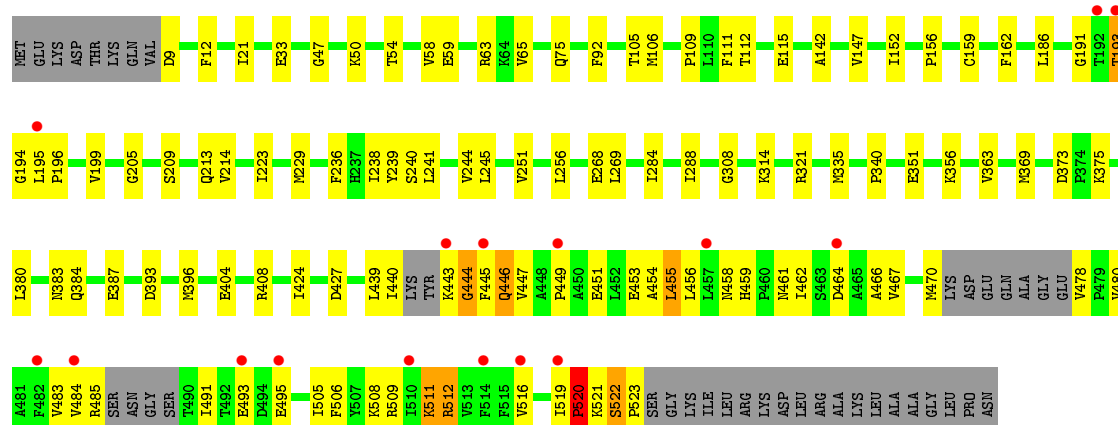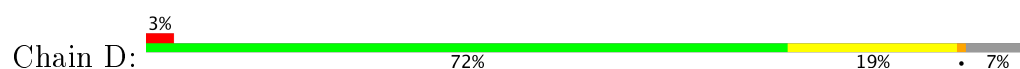- Molecule 1: 4-coumarate–CoA ligase 2

- Molecule 1: 4-coumarate–CoA ligase 2

• Molecule 1: 4-coumarate–CoA ligase 2

Chain D:
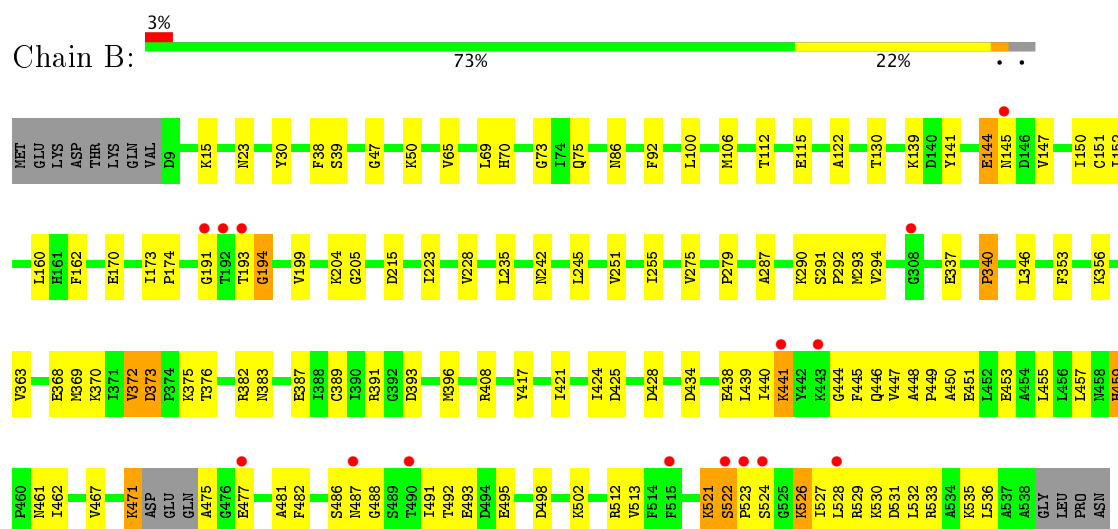
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	108.26Å 108.26Å 183.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.41 – 2.25 48.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.41-2.25) 98.2 (48.41-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.24Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.193 , 0.260 0.192 , 0.259	Depositor DCC
R_{free} test set	1936 reflections (1.98%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15622	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.74 % 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 4.3922e-03.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: 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	A	0.47	0/3328	0.61	2/4520 (0.0%)
1	B	0.46	1/4138 (0.0%)	0.67	2/5615 (0.0%)
1	C	0.44	0/4107	0.66	2/5568 (0.0%)
1	D	0.51	2/3949 (0.1%)	0.68	1/5363 (0.0%)
All	All	0.47	3/15522 (0.0%)	0.66	7/21066 (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
1	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	520	PRO	N-CD	-10.67	1.32	1.47
1	D	21	ILE	C-N	-6.45	1.22	1.34
1	B	372	VAL	C-N	-5.46	1.21	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	373	ASP	CB-CG-OD2	-8.59	110.57	118.30
1	B	441	LYS	CD-CE-NZ	-8.14	92.98	111.70
1	A	250	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	533	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	D	455	LEU	CA-CB-CG	5.64	128.28	115.30
1	C	512	ARG	NE-CZ-NH2	-5.19	117.70	120.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	467	VAL	Peptide
1	C	477	GLU	Peptide

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	3260	0	3290	38	0
1	B	4055	0	4129	103	0
1	C	4028	0	4098	92	0
1	D	3869	0	3924	87	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	129	0	0	2	1
3	B	69	0	0	3	0
3	C	81	0	0	8	0
3	D	126	0	0	9	1
All	All	15622	0	15441	317	1

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 10.

All (317) 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:522:SER:CB	1:B:526:LYS:HD3	1.88	1.03
1:A:19:ILE:H	1:A:366:ASN:HD21	1.22	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:HG13	1:C:396:MET:HE3	1.55	0.86
1:C:509:ARG:NH2	3:C:702:HOH:O	2.08	0.85
1:D:47:GLY:O	1:D:50:LYS:NZ	2.10	0.84
1:D:519:ILE:HG22	1:D:520:PRO:HD2	1.57	0.84
1:C:478:VAL:HG13	1:C:511:LYS:HG3	1.59	0.84
1:C:512:ARG:NH2	1:D:321:ARG:O	2.12	0.83
1:D:63:ARG:NH1	3:D:701:HOH:O	2.08	0.83
1:C:441:LYS:HG3	1:C:477:GLU:HB3	1.60	0.82
1:C:452:LEU:O	1:C:456:LEU:HD12	1.80	0.81
1:C:469:PRO:HD2	1:C:533:ARG:HH21	1.47	0.80
1:B:408:ARG:HH12	1:B:527:ILE:H	1.29	0.80
1:D:199:VAL:HG13	1:D:396:MET:HE3	1.63	0.80
1:B:524:SER:HB2	1:B:526:LYS:HD2	1.64	0.80
1:B:373:ASP:OD2	1:B:375:LYS:HG2	1.82	0.79
1:B:86:ASN:HD21	1:B:235:LEU:H	1.32	0.78
1:D:519:ILE:CG2	1:D:520:PRO:HD2	2.14	0.78
1:B:23:ASN:HB2	1:B:204:LYS:HG3	1.66	0.78
1:B:47:GLY:O	1:B:50:LYS:NZ	2.17	0.78
1:B:522:SER:HB2	1:B:526:LYS:HD3	1.64	0.77
1:C:485:ARG:NH1	1:C:491:ILE:O	2.18	0.77
1:B:363:VAL:HB	1:B:369:MET:HE1	1.68	0.76
1:C:529:ARG:HB3	1:C:533:ARG:HH12	1.49	0.76
1:D:195:LEU:HG	1:D:196:PRO:HD2	1.70	0.74
1:C:368:GLU:OE1	3:C:701:HOH:O	2.05	0.74
1:A:271:GLN:HE21	1:A:298:ASP:H	1.34	0.73
1:D:59:GLU:OE1	3:D:701:HOH:O	2.05	0.73
1:D:363:VAL:HB	1:D:369:MET:HE1	1.70	0.72
1:C:529:ARG:CZ	1:C:533:ARG:HH22	2.03	0.72
1:C:19:ILE:H	1:C:366:ASN:HD21	1.36	0.72
1:B:522:SER:OG	1:B:526:LYS:HD3	1.90	0.71
1:D:373:ASP:HB2	1:D:380:LEU:HD21	1.73	0.71
3:A:770:HOH:O	1:B:293:MET:SD	2.50	0.70
1:D:387:GLU:OE2	3:D:702:HOH:O	2.09	0.69
1:B:122:ALA:O	3:B:701:HOH:O	2.11	0.68
1:C:469:PRO:HD2	1:C:533:ARG:HE	1.59	0.68
1:D:454:ALA:O	1:D:458:ASN:ND2	2.24	0.68
1:C:441:LYS:CG	1:C:477:GLU:HB3	2.24	0.68
1:B:356:LYS:NZ	1:B:425:ASP:OD2	2.26	0.67
1:D:75:GLN:NE2	3:D:707:HOH:O	2.26	0.67
1:D:33:GLU:OE2	3:D:703:HOH:O	2.12	0.67
1:D:9:ASP:N	3:D:709:HOH:O	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:HIS:HB3	1:B:462:ILE:HD12	1.76	0.67
1:B:522:SER:HB2	1:B:526:LYS:HZ2	1.60	0.66
1:D:478:VAL:HG11	1:D:511:LYS:HD3	1.77	0.66
1:D:493:GLU:OE2	1:D:512:ARG:HD3	1.96	0.66
1:C:223:ILE:HG13	1:C:251:VAL:HG21	1.76	0.66
1:D:268:GLU:OE2	3:D:704:HOH:O	2.14	0.66
1:A:271:GLN:NE2	1:A:298:ASP:H	1.94	0.65
1:C:469:PRO:CD	1:C:533:ARG:HH21	2.09	0.65
1:C:478:VAL:CG1	1:C:511:LYS:HG3	2.27	0.65
1:C:469:PRO:HD2	1:C:533:ARG:NH2	2.12	0.65
1:C:527:ILE:HG22	1:C:529:ARG:HG2	1.78	0.65
1:C:112:THR:OG1	1:C:115:GLU:HG3	1.97	0.64
1:D:363:VAL:HB	1:D:369:MET:CE	2.27	0.64
1:D:443:LYS:HG2	1:D:444:GLY:N	2.12	0.64
1:C:461:ASN:HD22	1:C:491:ILE:HD11	1.61	0.64
1:C:478:VAL:HG13	1:C:511:LYS:CG	2.28	0.64
1:B:191:GLY:HA2	1:B:337:GLU:OE1	1.98	0.63
1:D:112:THR:OG1	1:D:115:GLU:HG2	1.98	0.63
1:B:482:PHE:HZ	1:B:536:LEU:HD21	1.62	0.63
1:B:492:THR:HG23	1:B:495:GLU:H	1.63	0.63
1:D:199:VAL:HG13	1:D:396:MET:CE	2.27	0.62
1:B:439:LEU:HD11	1:B:448:ALA:HA	1.81	0.62
1:C:449:PRO:O	1:C:453:GLU:HG3	2.01	0.61
1:B:461:ASN:HB2	1:B:491:ILE:HD11	1.82	0.60
1:B:446:GLN:N	1:B:446:GLN:OE1	2.34	0.60
1:B:522:SER:HB2	1:B:526:LYS:NZ	2.16	0.60
1:B:373:ASP:OD2	1:B:376:THR:N	2.31	0.60
1:B:471:LYS:HZ3	1:B:475:ALA:HB3	1.67	0.60
1:D:485:ARG:HG2	1:D:491:ILE:HG21	1.84	0.60
1:A:223:ILE:HG13	1:A:251:VAL:HG21	1.84	0.59
1:D:519:ILE:HG22	1:D:520:PRO:CD	2.30	0.59
1:B:528:LEU:O	1:B:531:ASP:HB2	2.02	0.59
1:C:356:LYS:NZ	1:C:427:ASP:OD2	2.35	0.59
1:C:469:PRO:HD2	1:C:533:ARG:NE	2.18	0.59
1:D:111:PHE:HB3	1:D:115:GLU:HG3	1.83	0.59
1:B:451:GLU:O	1:B:455:LEU:HD13	2.03	0.59
1:D:447:VAL:HG22	1:D:508:LYS:HB3	1.85	0.59
1:D:356:LYS:NZ	1:D:427:ASP:OD2	2.36	0.59
1:D:443:LYS:HE3	1:D:445:PHE:CD1	2.39	0.58
1:B:141:TYR:O	1:B:144:GLU:HG3	2.02	0.58
1:B:112:THR:OG1	1:B:115:GLU:HG3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LYS:HD2	1:C:168:ALA:O	2.03	0.58
1:D:443:LYS:O	1:D:445:PHE:N	2.36	0.58
1:D:453:GLU:HG2	1:D:467:VAL:HG23	1.84	0.58
1:A:140:ASP:O	1:A:144:GLU:HG3	2.03	0.58
1:B:73:GLY:O	1:B:75:GLN:NE2	2.24	0.57
1:B:86:ASN:ND2	1:B:235:LEU:H	2.00	0.57
1:B:493:GLU:OE2	3:B:702:HOH:O	2.17	0.57
1:C:23:ASN:HB2	1:C:204:LYS:HG3	1.86	0.57
1:D:223:ILE:HG13	1:D:251:VAL:HG21	1.86	0.57
1:D:505:ILE:HG22	1:D:508:LYS:HE2	1.86	0.57
1:C:453:GLU:HG2	1:C:467:VAL:HG13	1.86	0.57
1:D:284:ILE:O	1:D:288:ILE:HG13	2.04	0.57
1:D:256:LEU:HD21	1:D:269:LEU:HB3	1.88	0.56
1:B:287:ALA:HA	1:B:290:LYS:HE3	1.86	0.56
1:B:145:ASN:HB3	1:B:147:VAL:HG23	1.88	0.56
1:C:500:ILE:HG13	1:C:510:ILE:HD12	1.87	0.56
1:B:449:PRO:HB3	1:B:467:VAL:HG22	1.88	0.56
1:C:412:LYS:HD3	1:C:412:LYS:N	2.21	0.56
1:C:441:LYS:HG2	1:C:477:GLU:OE1	2.06	0.56
1:D:485:ARG:NH2	1:D:516:VAL:O	2.31	0.56
1:C:490:THR:O	1:C:491:ILE:HD12	2.06	0.55
1:B:439:LEU:HD12	1:B:449:PRO:HD2	1.88	0.55
1:B:369:MET:HG3	1:B:389:CYS:O	2.07	0.55
1:C:529:ARG:NH1	1:C:533:ARG:HH22	2.04	0.55
1:A:85:PRO:HB2	1:A:259:GLN:HG3	1.89	0.55
1:C:467:VAL:O	1:C:529:ARG:NH2	2.40	0.54
1:A:320:VAL:HG11	1:A:329:LEU:HD13	1.89	0.54
1:B:453:GLU:OE1	1:B:529:ARG:NH2	2.34	0.54
1:B:482:PHE:CZ	1:B:536:LEU:HD21	2.42	0.54
1:A:365:ARG:HG3	1:A:366:ASN:HD22	1.72	0.54
1:B:279:PRO:HG2	3:B:723:HOH:O	2.08	0.54
1:C:238:ILE:HG23	1:C:340:PRO:HG3	1.91	0.53
1:D:194:GLY:HA2	1:D:451:GLU:HG2	1.89	0.53
1:B:363:VAL:HB	1:B:369:MET:CE	2.38	0.53
1:B:493:GLU:HG3	1:B:513:VAL:CG1	2.38	0.53
1:C:331:GLN:OE1	3:C:703:HOH:O	2.18	0.53
1:B:15:LYS:HD2	1:B:428:ASP:HB2	1.91	0.53
1:A:161:HIS:CD2	1:A:163:SER:H	2.27	0.53
1:D:156:PRO:HG2	1:D:159:CYS:SG	2.50	0.53
1:B:449:PRO:O	1:B:453:GLU:HG3	2.09	0.52
1:C:195:LEU:HD11	1:C:451:GLU:HA	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:THR:HB	1:B:450:ALA:CB	2.40	0.52
1:B:522:SER:HB2	1:B:526:LYS:CD	2.38	0.52
1:C:529:ARG:O	1:C:532:LEU:N	2.43	0.52
1:D:239:TYR:CZ	1:D:308:GLY:HA2	2.45	0.52
1:B:290:LYS:HG2	1:B:290:LYS:O	2.09	0.52
1:C:373:ASP:HB2	1:C:380:LEU:HD11	1.92	0.52
1:D:447:VAL:HG21	1:D:508:LYS:HA	1.92	0.52
1:C:485:ARG:HH11	1:C:491:ILE:H	1.56	0.52
1:A:127:ILE:HG21	1:A:150:ILE:HD12	1.92	0.51
1:C:376:THR:HG23	1:C:378:ASN:H	1.75	0.51
1:D:351:GLU:HA	1:D:351:GLU:OE2	2.11	0.51
1:B:291:SER:HB3	1:B:294:VAL:HG23	1.93	0.51
1:C:529:ARG:HB3	1:C:533:ARG:NH1	2.23	0.51
1:D:240:SER:HB2	3:D:779:HOH:O	2.10	0.51
1:A:208:THR:O	1:A:212:GLN:HG3	2.11	0.50
1:B:523:PRO:HD2	1:B:526:LYS:HZ3	1.75	0.50
1:C:493:GLU:HG3	1:C:513:VAL:HB	1.92	0.50
1:D:522:SER:HB2	1:D:523:PRO:HD2	1.92	0.50
1:C:291:SER:HB3	1:C:294:VAL:HG23	1.94	0.50
1:C:479:PRO:HG2	1:C:509:ARG:O	2.12	0.50
1:C:175:GLU:H	1:C:175:GLU:CD	2.15	0.50
1:A:339:GLY:N	1:A:340:PRO:HA	2.27	0.50
1:B:498:ASP:O	1:B:502:LYS:HG2	2.12	0.50
1:C:422:GLY:HA3	3:C:746:HOH:O	2.10	0.50
1:B:370:LYS:HE3	1:B:372:VAL:HG11	1.94	0.49
1:C:468:VAL:HA	1:C:533:ARG:NH2	2.27	0.49
1:C:470:MET:HG2	1:C:471:LYS:N	2.25	0.49
1:D:485:ARG:HG3	1:D:485:ARG:HH11	1.77	0.49
1:D:461:ASN:O	1:D:485:ARG:HA	2.12	0.49
1:C:464:ASP:HB3	1:C:519:ILE:HD11	1.95	0.49
1:C:511:LYS:O	1:C:512:ARG:HG2	2.12	0.49
1:A:43:CYS:SG	1:A:58:VAL:HG21	2.53	0.49
1:B:523:PRO:HD2	1:B:526:LYS:NZ	2.28	0.49
1:B:486:SER:O	1:B:488:GLY:N	2.41	0.49
1:D:373:ASP:OD2	1:D:375:LYS:HB2	2.13	0.49
1:B:383:ASN:ND2	1:B:425:ASP:HA	2.27	0.48
1:C:469:PRO:HD2	1:C:533:ARG:CZ	2.43	0.48
1:B:532:LEU:O	1:B:536:LEU:HG	2.13	0.48
1:C:453:GLU:CG	1:C:467:VAL:HG13	2.43	0.48
1:A:233:LEU:HB2	1:A:240:SER:OG	2.14	0.48
1:A:265:SER:HA	1:A:268:GLU:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:VAL:HG11	1:C:336:THR:HG22	1.96	0.48
1:B:245:LEU:HD12	1:B:255:ILE:HD13	1.96	0.48
1:D:446:GLN:O	1:D:447:VAL:HG23	2.13	0.48
1:A:50:LYS:HD2	1:A:273:TYR:OH	2.13	0.48
1:B:523:PRO:HG2	1:B:526:LYS:NZ	2.29	0.48
1:A:160:LEU:HA	1:D:383:ASN:HB3	1.96	0.47
1:A:118:LYS:NZ	1:A:196:PRO:HG2	2.29	0.47
1:D:9:ASP:N	3:D:718:HOH:O	2.46	0.47
1:B:372:VAL:HG21	1:B:417:TYR:CE1	2.49	0.47
1:A:64:LYS:HD3	1:A:166:THR:O	2.14	0.47
1:B:193:THR:OG1	1:B:194:GLY:N	2.46	0.47
1:C:492:THR:HG23	1:C:495:GLU:H	1.78	0.47
1:D:470:MET:SD	1:D:480:VAL:HG21	2.54	0.47
1:B:368:GLU:OE2	1:B:391:ARG:NH2	2.44	0.47
1:C:440:ILE:HG12	1:C:447:VAL:O	2.14	0.47
1:D:480:VAL:HG22	1:D:512:ARG:HB3	1.97	0.47
1:A:346:LEU:HB3	1:A:353:PHE:HB2	1.96	0.46
1:C:439:LEU:HD13	1:C:447:VAL:O	2.15	0.46
1:D:439:LEU:O	1:D:439:LEU:HG	2.15	0.46
1:B:372:VAL:HG21	1:B:417:TYR:HE1	1.80	0.46
1:C:239:TYR:CZ	1:C:308[A]:GLY:HA3	2.50	0.46
1:C:12:PHE:CD1	1:C:424:ILE:HD12	2.50	0.46
1:D:241:LEU:HD12	1:D:245:LEU:HD23	1.98	0.46
1:D:65:VAL:HG21	1:D:92:PHE:HB3	1.97	0.46
1:B:493:GLU:HG3	1:B:513:VAL:HG12	1.97	0.46
1:C:529:ARG:NH1	1:C:533:ARG:NH2	2.62	0.46
1:C:189:SER:O	1:C:196:PRO:HA	2.15	0.46
1:D:446:GLN:C	1:D:447:VAL:HG23	2.36	0.46
1:B:441:LYS:O	1:B:477:GLU:HB3	2.15	0.46
1:B:65:VAL:HG21	1:B:92:PHE:HB3	1.97	0.46
1:C:455:LEU:HD22	1:C:503:GLN:OE1	2.16	0.46
1:D:105:THR:HB	1:D:186:LEU:HD23	1.98	0.46
1:D:519:ILE:O	1:D:521:LYS:N	2.48	0.46
1:C:391:ARG:NH2	3:C:701:HOH:O	2.49	0.46
1:B:530:LYS:HG3	1:B:533:ARG:HD3	1.97	0.45
1:B:30:TYR:OH	1:B:215:ASP:OD1	2.22	0.45
1:C:11:ILE:HD13	3:C:701:HOH:O	2.17	0.45
1:D:521:LYS:HD2	1:D:521:LYS:HA	1.88	0.45
1:C:471:LYS:HE2	1:C:474:GLN:HB2	1.99	0.45
1:D:12:PHE:CD2	1:D:424:ILE:HD12	2.52	0.45
1:B:373:ASP:OD2	1:B:375:LYS:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:MET:O	1:C:471:LYS:HB3	2.17	0.45
1:D:142:ALA:HB1	1:D:147:VAL:O	2.16	0.45
1:D:462:ILE:HG23	1:D:483:VAL:HB	1.98	0.45
1:B:382:ARG:HB3	1:B:424:ILE:O	2.16	0.45
1:C:477:GLU:O	1:C:478:VAL:HG23	2.17	0.45
1:A:55:TYR:CZ	1:A:252:GLY:HA2	2.52	0.45
1:B:145:ASN:CB	1:B:147:VAL:HG23	2.47	0.45
1:B:439:LEU:CD1	1:B:448:ALA:HA	2.47	0.45
1:C:469:PRO:HB3	1:C:477:GLU:CD	2.37	0.45
1:C:471:LYS:CE	1:C:474:GLN:HB2	2.47	0.45
1:B:139:LYS:O	1:B:139:LYS:HD3	2.17	0.44
1:B:160:LEU:HA	1:C:383:ASN:HB3	1.99	0.44
1:B:453:GLU:CG	1:B:467:VAL:HG13	2.46	0.44
1:C:190:SER:HB2	1:C:194:GLY:O	2.17	0.44
1:B:492:THR:OG1	1:B:493:GLU:N	2.50	0.44
1:C:245:LEU:HD12	1:C:255:ILE:HD13	1.99	0.44
1:C:370:LYS:HE3	1:C:372:VAL:HG21	1.98	0.44
1:B:522:SER:CB	1:B:526:LYS:CD	2.78	0.44
1:C:24:HIS:HB2	3:C:762:HOH:O	2.17	0.44
1:D:404:GLU:O	1:D:408:ARG:HG3	2.18	0.44
1:B:453:GLU:O	1:B:457:LEU:HD23	2.17	0.44
1:C:30:TYR:OH	1:C:215:ASP:OD2	2.23	0.44
1:D:446:GLN:O	1:D:447:VAL:CG2	2.66	0.44
1:A:156:PRO:HD2	1:A:159:CYS:HB2	2.00	0.44
1:C:464:ASP:HB3	1:C:519:ILE:CD1	2.48	0.44
1:D:238:ILE:HG23	1:D:340:PRO:HG3	1.99	0.44
1:B:199:VAL:HG13	1:B:396:MET:HE3	1.99	0.43
1:B:441:LYS:HD2	1:B:441:LYS:HA	1.81	0.43
1:B:526:LYS:O	1:B:526:LYS:HG2	2.18	0.43
1:B:70:HIS:ND1	1:B:174:PRO:HG3	2.33	0.43
1:C:200:MET:CE	1:C:397:LYS:HD2	2.48	0.43
1:D:214:VAL:HG11	1:D:223:ILE:HD11	1.99	0.43
1:B:453:GLU:HG3	1:B:467:VAL:HG13	2.00	0.43
1:C:441:LYS:O	1:C:441:LYS:HG3	2.18	0.43
1:A:142:ALA:HB3	1:A:149:ILE:HD11	1.99	0.43
1:D:191:GLY:C	1:D:193:THR:H	2.22	0.43
1:B:242:ASN:ND2	1:B:340:PRO:HD2	2.33	0.43
1:A:136:ASN:N	3:A:721:HOH:O	2.52	0.43
1:B:369:MET:HE3	1:B:424:ILE:HD11	2.00	0.43
1:D:268:GLU:HA	1:D:268:GLU:OE1	2.19	0.43
1:B:223:ILE:HG13	1:B:251:VAL:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ARG:NH2	1:C:225:SER:O	2.52	0.42
1:C:477:GLU:HG2	1:C:478:VAL:H	1.83	0.42
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.82	0.42
1:B:69:LEU:HB2	1:B:100:LEU:HD11	2.01	0.42
1:B:440:ILE:HB	1:B:447:VAL:HB	2.00	0.42
1:A:9:ASP:OD1	1:A:9:ASP:N	2.53	0.42
1:B:130:THR:O	1:B:151:CYS:HA	2.19	0.42
1:B:205:GLY:HA2	1:B:393:ASP:O	2.20	0.42
1:D:152:ILE:HA	1:D:162:PHE:HB2	2.00	0.42
1:A:409:THR:HG22	1:A:416:LEU:CD1	2.50	0.42
1:B:461:ASN:HB2	1:B:491:ILE:CD1	2.48	0.42
1:C:437:LYS:HB3	1:C:438:GLU:H	1.65	0.42
1:A:161:HIS:HD2	1:A:163:SER:OG	2.02	0.42
1:B:481:ALA:O	1:B:513:VAL:HA	2.20	0.42
1:D:447:VAL:CG2	1:D:508:LYS:HA	2.50	0.42
1:B:421:ILE:HB	1:B:434:ASP:HB3	2.02	0.42
1:B:438:GLU:HG2	1:B:439:LEU:N	2.35	0.42
1:C:346:LEU:HB3	1:C:353:PHE:HB2	2.00	0.42
1:C:529:ARG:O	1:C:532:LEU:HB2	2.20	0.42
1:D:485:ARG:NH1	1:D:485:ARG:HG3	2.35	0.42
1:B:152:ILE:HA	1:B:162:PHE:HB2	2.01	0.42
1:C:468:VAL:HG12	1:C:469:PRO:O	2.20	0.41
1:D:205:GLY:HA2	1:D:393:ASP:O	2.20	0.41
1:D:335:MET:O	1:D:340:PRO:HA	2.18	0.41
1:D:54:THR:O	1:D:58:VAL:HG23	2.19	0.41
1:A:197:LYS:HB3	1:A:399:TYR:CD1	2.55	0.41
1:A:373:ASP:HA	1:A:374:PRO:HD3	1.91	0.41
1:A:84:LEU:HD22	1:A:152:ILE:HD13	2.01	0.41
1:B:228:VAL:HB	1:B:275:VAL:HA	2.01	0.41
1:D:440:ILE:HD12	1:D:449:PRO:HD3	2.02	0.41
1:B:521:LYS:HG2	1:B:527:ILE:CD1	2.50	0.41
1:C:11:ILE:CG2	1:C:368:GLU:HB3	2.50	0.41
1:D:115:GLU:H	1:D:115:GLU:HG2	1.66	0.41
1:D:380:LEU:HD13	1:D:384:GLN:HG2	2.01	0.41
1:D:478:VAL:CG1	1:D:511:LYS:HD3	2.48	0.41
1:B:372:VAL:O	1:B:387:GLU:N	2.48	0.41
1:C:129:VAL:HA	1:C:150:ILE:O	2.20	0.41
1:D:229:MET:HE2	1:D:244:VAL:HG13	2.01	0.41
1:D:483:VAL:O	1:D:485:ARG:NH1	2.53	0.41
1:A:373:ASP:OD2	1:A:376:THR:HG23	2.20	0.41
1:D:453:GLU:CD	1:D:466:ALA:HA	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HA	1:B:160:LEU:O	2.21	0.41
1:C:43:CYS:HB2	1:C:55:TYR:CD1	2.56	0.41
1:D:464:ASP:HB3	1:D:484:VAL:HG11	2.03	0.41
1:D:506:PHE:HA	1:D:509:ARG:NE	2.35	0.41
1:D:209:SER:O	1:D:213:GLN:HG3	2.20	0.41
1:A:161:HIS:HD2	1:A:163:SER:CB	2.34	0.41
1:A:412:LYS:H	1:A:412:LYS:HG3	1.72	0.41
1:B:170:GLU:O	1:B:173:ILE:HG13	2.20	0.41
1:C:365:ARG:HG3	1:C:366:ASN:HD22	1.84	0.41
1:D:443:LYS:HE2	1:D:443:LYS:HB3	1.44	0.41
1:D:491:ILE:HG13	1:D:495:GLU:OE1	2.20	0.41
1:A:135:VAL:HG12	1:A:139:LYS:HB2	2.02	0.41
1:B:292:PRO:HD2	1:B:293:MET:HE3	2.03	0.41
1:A:333:TYR:OH	1:A:420:ASP:OD2	2.23	0.40
1:B:15:LYS:HE2	1:B:353:PHE:CD1	2.56	0.40
1:B:445:PHE:HA	1:B:446:GLN:OE1	2.21	0.40
1:A:370:LYS:HE3	1:A:372:VAL:CG2	2.51	0.40
1:B:346:LEU:HA	1:B:346:LEU:HD23	1.90	0.40
1:B:493:GLU:HG3	1:B:513:VAL:HG13	2.03	0.40
1:C:169:ASN:ND2	1:C:171:HIS:H	2.19	0.40
1:C:290:LYS:O	1:C:290:LYS:HG2	2.21	0.40
1:B:521:LYS:HG2	1:B:527:ILE:HD13	2.02	0.40
1:D:109:PRO:HD2	1:D:236:PHE:CE2	2.56	0.40
1:C:432:ILE:HG12	3:C:746:HOH:O	2.22	0.40
1:A:373:ASP:HB2	1:A:380:LEU:HD21	2.04	0.40
1:C:483:VAL:O	1:C:515:PHE:HA	2.21	0.40
1:D:439:LEU:CG	1:D:439:LEU:O	2.70	0.40
1:D:456:LEU:HD22	1:D:483:VAL:HG11	2.04	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
3:A:704:HOH:O	3:D:772:HOH:O[3_555]	2.12	0.08

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	420/542 (78%)	403 (96%)	17 (4%)	0	100	100
1	B	523/542 (96%)	492 (94%)	25 (5%)	6 (1%)	17	12
1	C	513/542 (95%)	482 (94%)	26 (5%)	5 (1%)	18	15
1	D	494/542 (91%)	468 (95%)	22 (4%)	4 (1%)	22	20
All	All	1950/2168 (90%)	1845 (95%)	90 (5%)	15 (1%)	22	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	521	LYS
1	D	444	GLY
1	C	193	THR
1	C	309	ALA
1	C	437	LYS
1	D	520	PRO
1	B	194	GLY
1	B	487	ASN
1	C	444	GLY
1	C	528	LEU
1	D	193	THR
1	B	522	SER
1	B	444	GLY
1	B	535	LYS
1	D	522	SER

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	363/463 (78%)	356 (98%)	7 (2%)	62	72
1	B	449/463 (97%)	440 (98%)	9 (2%)	60	70
1	C	445/463 (96%)	436 (98%)	9 (2%)	60	70
1	D	431/463 (93%)	424 (98%)	7 (2%)	68	78
All	All	1688/1852 (91%)	1656 (98%)	32 (2%)	62	72

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	38	PHE
1	A	62	SER
1	A	69	LEU
1	A	106	MET
1	A	189	SER
1	A	357	SER
1	B	38	PHE
1	B	39	SER
1	B	106	MET
1	B	144	GLU
1	B	340	PRO
1	B	459	HIS
1	B	471	LYS
1	B	512	ARG
1	B	526	LYS
1	C	13	ARG
1	C	38	PHE
1	C	39	SER
1	C	106	MET
1	C	169	ASN
1	C	174	PRO
1	C	459	HIS
1	C	517	ASP
1	C	528	LEU
1	D	106	MET
1	D	314	LYS
1	D	446	GLN
1	D	455	LEU
1	D	459	HIS
1	D	511	LYS

Continued on next page...

Full wwPDB X-ray Structure Validation Report	5U95

Continued from previous page...

Mol	Chain	Res	Type
1	D	512	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	271	GLN
1	A	366	ASN
1	A	384	GLN
1	B	86	ASN
1	B	383	ASN
1	C	169	ASN
1	C	366	ASN
1	D	169	ASN
1	D	384	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 5 ligands modelled in this entry, 5 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)

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, 95th 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^2)	Q<0.9
1	A	424/542 (78%)	-0.24	2 (0%)	90	91	22, 39, 67, 101	0
1	B	527/542 (97%)	0.06	15 (2%)	53	57	30, 53, 104, 151	0
1	C	522/542 (96%)	0.05	23 (4%)	35	38	31, 52, 101, 152	0
1	D	502/542 (92%)	-0.03	16 (3%)	48	52	24, 44, 108, 161	0
All	All	1975/2168 (91%)	-0.03	56 (2%)	53	57	22, 48, 101, 161	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	THR	7.4
1	D	192	THR	6.4
1	D	493	GLU	6.3
1	C	520	PRO	5.4
1	D	193	THR	5.1
1	C	534	ALA	4.9
1	C	519	ILE	4.8
1	C	533	ARG	4.6
1	C	474	GLN	4.4
1	B	524	SER	4.4
1	C	443	LYS	4.3
1	B	487	ASN	3.6
1	B	523	PRO	3.6
1	C	525	GLY	3.6
1	C	460	PRO	3.5
1	C	530	LYS	3.3
1	C	490	THR	3.3
1	D	514	PHE	3.3
1	B	515	PHE	3.2
1	B	528	LEU	3.0
1	B	522	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	145	ASN	2.9
1	C	489	SER	2.9
1	C	518	ALA	2.9
1	D	457	LEU	2.8
1	C	441	LYS	2.8
1	C	536	LEU	2.8
1	C	483	VAL	2.8
1	D	519	ILE	2.8
1	D	484	VAL	2.7
1	B	477	GLU	2.7
1	C	308[A]	GLY	2.7
1	C	309	ALA	2.6
1	D	443	LYS	2.6
1	D	445	PHE	2.6
1	D	482	PHE	2.5
1	C	442	TYR	2.5
1	B	191	GLY	2.5
1	C	532	LEU	2.5
1	B	308	GLY	2.5
1	C	537	ALA	2.4
1	D	510	ILE	2.3
1	C	488	GLY	2.3
1	D	195	LEU	2.3
1	D	495	GLU	2.3
1	D	516	VAL	2.3
1	C	475	ALA	2.3
1	C	484	VAL	2.2
1	B	490	THR	2.2
1	B	443	LYS	2.2
1	D	464	ASP	2.1
1	D	449	PRO	2.1
1	B	193	THR	2.1
1	A	143	PHE	2.1
1	A	156	PRO	2.0
1	B	441	LYS	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	D	601	1/1	0.08	0.72	30.91	178,178,178,178	0
2	CA	A	601	1/1	0.92	0.19	5.70	42,42,42,42	0
2	CA	A	602	1/1	0.68	0.22	2.46	122,122,122,122	0
2	CA	C	601	1/1	0.84	0.19	1.76	111,111,111,111	0
2	CA	B	601	1/1	0.85	0.12	-0.48	62,62,62,62	0

6.5 Other polymers (i)

There are no such residues in this entry.