Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1XXD
Title	:	Crystal Structure of the FXIa Catalytic Domain in Complex with mutated Ecotin
Authors	:	Jin, L.; Pandey, P.; Babine, R.E.; Gorga, J.C.; Seidl, K.J.; Gelfand, E.; Weaver, D.T.; Abdel-Meguid, S.S.; Strickler, J.E.
Deposited on	:	2004-11-04
Resolution	:	2.91 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 (1)) were used in the production of this report:

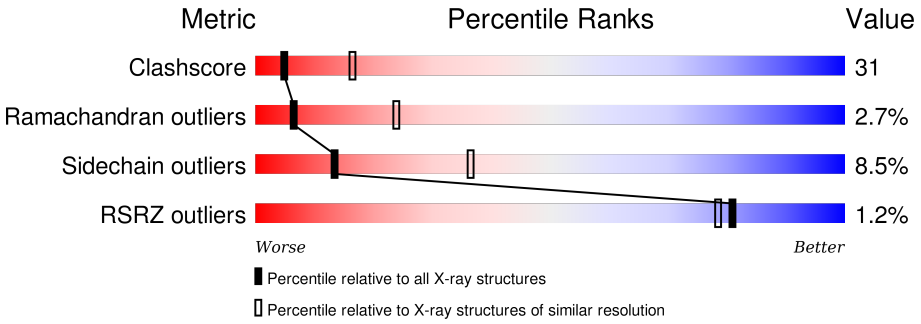
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1871 (2.94-2.90)
Ramachandran outliers	100387	1824 (2.94-2.90)
Sidechain outliers	100360	1826 (2.94-2.90)
RSRZ outliers	91569	1650 (2.94-2.90)

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	238	46% 49% 5%
1	B	238	% 51% 41% 8%
2	C	142	3% 42% 49% 5%
2	D	142	% 45% 42% 7% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6021 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 Coagulation factor XI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1885	1191	334	349	11			
1	B	238	Total	C	N	O	S	0	0	0
			1885	1191	334	349	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	56	ALA	SER	ENGINEERED	UNP P03951
A	97	ALA	THR	ENGINEERED	UNP P03951
B	56	ALA	SER	ENGINEERED	UNP P03951
B	97	ALA	THR	ENGINEERED	UNP P03951

- Molecule 2 is a protein called Ecotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	0
			1106	707	185	210	4			
2	D	134	Total	C	N	O	S	0	0	0
			1087	695	182	206	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	80	ASN	PRO	ENGINEERED	UNP P23827
C	81	ASP	VAL	ENGINEERED	UNP P23827
C	82	PHE	SER	ENGINEERED	UNP P23827
C	84	ARG	MET	ENGINEERED	UNP P23827
C	85	VAL	MET	ENGINEERED	UNP P23827
C	86	VAL	ALA	ENGINEERED	UNP P23827
D	80	ASN	PRO	ENGINEERED	UNP P23827
D	81	ASP	VAL	ENGINEERED	UNP P23827

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	82	PHE	SER	ENGINEERED	UNP P23827
D	84	ARG	MET	ENGINEERED	UNP P23827
D	85	VAL	MET	ENGINEERED	UNP P23827
D	86	VAL	ALA	ENGINEERED	UNP P23827

- Molecule 3 is water.

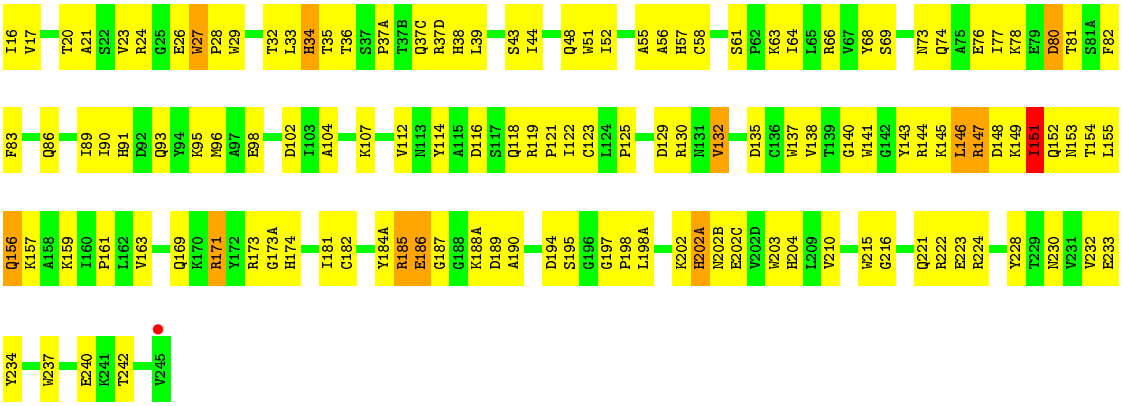
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	12	Total O 12 12	0	0
3	C	11	Total O 11 11	0	0
3	D	13	Total O 13 13	0	0

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

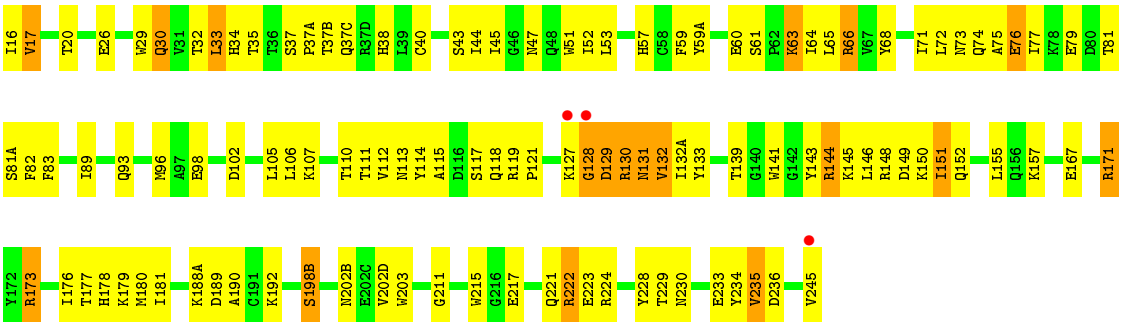
- Molecule 1: Coagulation factor XI

Chain A:



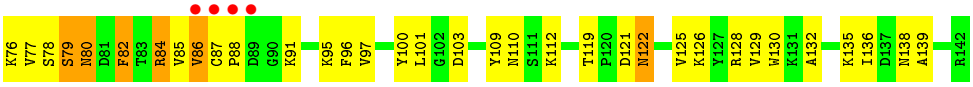
- Molecule 1: Coagulation factor XI

Chain B:

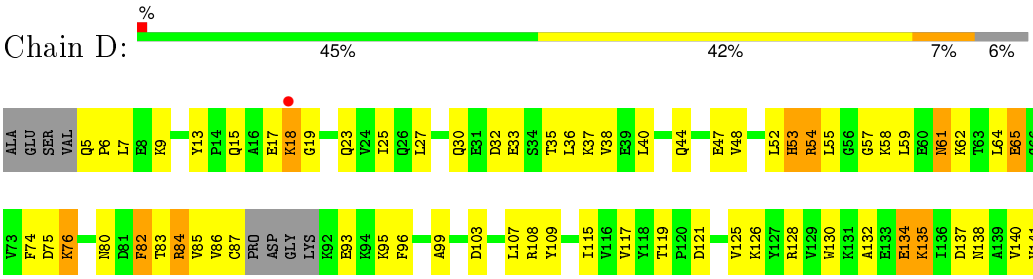


- Molecule 2: Ecotin

Chain C:



- Molecule 2: Ecotin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	45.45Å 91.42Å 188.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.91 44.18 – 2.91	Depositor EDS
% Data completeness (in resolution range)	87.6 (29.72-2.91) 87.6 (44.18-2.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.29 (at 2.90Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.230 , 0.282 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	48.8	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 16789 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6021	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.45	0/1930	0.66	0/2615
1	B	0.46	0/1930	0.64	0/2615
2	C	0.50	0/1128	0.67	0/1523
2	D	0.48	0/1107	0.66	0/1494
All	All	0.47	0/6095	0.66	0/8247

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	1885	0	1848	153	0
1	B	1885	0	1848	111	0
2	C	1106	0	1115	92	0
2	D	1087	0	1094	68	0
3	A	22	0	0	3	0
3	B	12	0	0	1	0
3	C	11	0	0	2	0
3	D	13	0	0	1	0
All	All	6021	0	5905	372	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 31.

All (372) 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:217:GLU:HG3	2:D:80:ASN:HD21	1.29	0.96
2:C:80:ASN:H	2:C:80:ASN:HD22	1.15	0.95
2:C:103:ASP:HB3	2:D:103:ASP:HB3	1.50	0.94
1:A:130:ARG:HH11	2:D:65:GLU:HG3	1.36	0.90
1:B:217:GLU:HG3	2:D:80:ASN:ND2	1.85	0.90
2:C:51:ASN:HB3	2:C:82:PHE:HB2	1.56	0.85
1:A:147:ARG:O	1:A:147:ARG:HG2	1.75	0.85
1:A:73:ASN:HA	1:A:153:ASN:O	1.77	0.82
2:C:80:ASN:N	2:C:80:ASN:HD22	1.73	0.81
1:A:129:ASP:HB3	1:A:132:VAL:HG11	1.63	0.81
1:B:173:ARG:HB3	2:D:76:LYS:HD3	1.63	0.80
1:A:16:ILE:HB	1:A:156:GLN:HB3	1.64	0.79
2:C:136:ILE:HD13	2:D:128:ARG:HB2	1.65	0.79
2:D:59:LEU:HD11	2:D:72:TYR:HB3	1.62	0.78
1:B:33:LEU:HD21	1:B:106:LEU:HD11	1.66	0.78
1:A:222:ARG:HH11	1:A:222:ARG:HG3	1.49	0.77
2:C:56:GLY:O	2:C:77:VAL:HA	1.84	0.77
1:B:96:MET:HE1	2:D:54:ARG:HB3	1.65	0.76
1:A:171:ARG:N	1:A:171:ARG:HD2	2.01	0.76
1:A:38:HIS:HB3	1:A:151:ILE:HD13	1.68	0.76
1:A:232:VAL:HG23	3:A:263:HOH:O	1.85	0.75
1:B:128:GLY:O	1:B:130:ARG:N	2.20	0.75
2:C:110:ASN:OD1	2:C:112:LYS:HB2	1.86	0.75
1:A:147:ARG:O	1:A:147:ARG:CG	2.34	0.74
2:C:19:GLY:O	2:C:20:MET:HG3	1.87	0.74
2:C:74:PHE:HB3	2:C:119:THR:HG22	1.68	0.74
1:A:35:THR:O	1:A:37(C):GLN:HA	1.90	0.72
1:B:127:LYS:O	1:B:128:GLY:O	2.07	0.72
1:A:114:TYR:CE1	1:A:121:PRO:HD3	2.24	0.72
2:C:37:LYS:HE2	2:D:130:TRP:CH2	2.24	0.72
2:C:132:ALA:HB1	2:D:128:ARG:HD3	1.72	0.71
1:B:177:THR:H	1:B:180:MET:HE3	1.53	0.71
1:A:73:ASN:HD22	1:A:154:THR:HA	1.54	0.71
2:D:25:ILE:HB	2:D:115:ILE:HB	1.72	0.71
1:A:156:GLN:HB2	3:A:255:HOH:O	1.89	0.71
2:D:40:LEU:HD11	2:D:107:LEU:HD11	1.73	0.71
1:B:176:ILE:HA	1:B:180:MET:HE3	1.72	0.70
2:D:72:TYR:HB2	2:D:117:VAL:HG22	1.72	0.70
1:B:129:ASP:OD1	1:B:129:ASP:O	2.09	0.69
1:B:167:GLU:OE1	1:B:171:ARG:NH2	2.26	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:48:VAL:HG12	2:C:52:LEU:HD13	1.73	0.69
1:A:215:TRP:C	2:C:84:ARG:NH1	2.45	0.69
2:C:8:GLU:N	2:C:8:GLU:OE1	2.25	0.69
1:B:217:GLU:CG	2:D:80:ASN:HD21	2.06	0.69
2:C:16:ALA:HB1	2:C:20:MET:O	1.92	0.68
2:D:57:GLY:HA2	2:D:76:LYS:O	1.92	0.68
2:C:6:PRO:HB2	2:C:9:LYS:HD2	1.75	0.68
1:A:43:SER:OG	1:A:198:PRO:HB3	1.93	0.68
2:C:48:VAL:HG11	2:C:52:LEU:HD22	1.75	0.68
1:A:215:TRP:C	2:C:84:ARG:HH11	1.97	0.68
1:B:73:ASN:O	1:B:76:GLU:HG2	1.93	0.68
1:B:132(A):ILE:O	1:B:132(A):ILE:HG13	1.93	0.68
2:C:80:ASN:N	2:C:80:ASN:ND2	2.43	0.67
1:B:131:ASN:OD1	1:B:131:ASN:C	2.33	0.67
1:B:111:THR:HG22	1:B:112:VAL:N	2.10	0.67
1:A:37(D):ARG:NH2	2:C:88:PRO:HD3	2.10	0.67
1:B:177:THR:H	1:B:180:MET:CE	2.08	0.67
1:A:98:GLU:N	1:A:98:GLU:OE1	2.24	0.66
1:B:96:MET:CE	2:D:54:ARG:HB3	2.24	0.66
1:A:184(A):TYR:O	1:A:187:GLY:N	2.28	0.66
1:A:73:ASN:ND2	1:A:154:THR:HA	2.11	0.65
2:D:48:VAL:HG12	2:D:52:LEU:HD23	1.78	0.65
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.61	0.65
2:C:49:ASP:CG	2:C:50:CYS:H	1.97	0.65
1:A:66:ARG:HG2	1:A:82:PHE:CE1	2.31	0.65
2:C:49:ASP:CG	2:C:50:CYS:N	2.49	0.64
1:A:73:ASN:HB3	1:A:153:ASN:OD1	1.96	0.64
2:C:11:ALA:HB3	2:C:13:TYR:CE2	2.32	0.64
2:C:74:PHE:CB	2:C:119:THR:HG22	2.26	0.64
1:B:146:LEU:O	1:B:148:ARG:HB2	1.97	0.64
1:A:138:VAL:HG23	1:A:138:VAL:O	1.98	0.64
1:A:48:GLN:O	1:A:48:GLN:HG2	1.97	0.63
1:A:173:ARG:O	2:C:58:LYS:HE3	1.98	0.63
2:C:42:ILE:HD12	2:C:101:LEU:HD11	1.79	0.63
1:B:211:GLY:HA2	1:B:229:THR:O	1.99	0.63
1:B:144:ARG:HG3	1:B:149:ASP:OD2	1.99	0.63
1:A:38:HIS:O	2:C:86:VAL:HG11	1.99	0.62
1:A:173:ARG:HG2	2:C:76:LYS:HE3	1.80	0.62
1:A:157:LYS:HG3	1:A:157:LYS:O	2.00	0.61
1:A:152:GLN:NE2	1:A:152:GLN:HA	2.15	0.61
1:B:114:TYR:HA	1:B:118:GLN:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:HG12	1:A:198(A):LEU:CD1	2.31	0.61
1:B:16:ILE:O	1:B:144:ARG:HA	2.00	0.61
1:B:30:GLN:NE2	1:B:139:THR:OG1	2.33	0.60
1:A:125:PRO:CB	1:A:232:VAL:HG22	2.31	0.60
1:A:68:TYR:CE2	1:A:77:ILE:HG23	2.35	0.60
1:B:61:SER:HB3	1:B:64:ILE:HG23	1.83	0.60
1:B:215:TRP:HB3	2:D:83:THR:HG22	1.83	0.60
1:A:151:ILE:O	1:A:151:ILE:HG22	2.00	0.60
1:A:240:GLU:HG2	2:D:67:TRP:HH2	1.67	0.60
1:A:55:ALA:HB3	1:A:58:CYS:SG	2.42	0.59
1:A:37(D):ARG:CZ	2:C:88:PRO:HD3	2.32	0.59
1:A:51:TRP:CE3	1:A:242:THR:HG22	2.36	0.59
1:A:230:ASN:ND2	1:A:233:GLU:HG2	2.17	0.59
1:B:132:VAL:HG13	1:B:133:TYR:CZ	2.37	0.59
1:B:26:GLU:N	3:B:257:HOH:O	2.24	0.59
1:A:26:GLU:HG2	1:A:27:TRP:CE2	2.37	0.59
2:D:86:VAL:C	2:D:87:CYS:SG	2.80	0.58
2:D:48:VAL:HB	2:D:52:LEU:HB3	1.84	0.58
1:B:68:TYR:CE2	1:B:82:PHE:HB3	2.37	0.58
2:C:130:TRP:CZ2	2:D:132:ALA:HB2	2.38	0.58
1:B:33:LEU:HD21	1:B:106:LEU:CD1	2.33	0.58
1:B:66:ARG:HD2	1:B:82:PHE:CE1	2.38	0.58
1:A:151:ILE:HD12	2:C:86:VAL:HG21	1.86	0.58
1:A:23:VAL:HG22	1:A:24:ARG:N	2.19	0.58
2:C:95:LYS:HG2	2:C:96:PHE:H	1.68	0.58
1:B:130:ARG:NH2	2:C:65:GLU:HG3	2.19	0.57
1:A:91:HIS:HE1	2:D:67:TRP:O	1.87	0.57
1:A:202:LYS:HB2	1:A:203:TRP:CZ2	2.39	0.57
1:B:130:ARG:HH21	2:C:65:GLU:HG3	1.68	0.57
1:A:144:ARG:NH1	1:A:152:GLN:NE2	2.52	0.57
1:A:26:GLU:HG2	1:A:27:TRP:NE1	2.20	0.57
1:B:75:ALA:O	1:B:77:ILE:N	2.38	0.57
2:C:52:LEU:HD22	2:C:97:VAL:HG11	1.87	0.57
1:A:38:HIS:HB3	1:A:151:ILE:CD1	2.34	0.57
2:C:128:ARG:HD3	2:D:132:ALA:HB1	1.86	0.57
2:C:7:LEU:HD23	2:C:22:ARG:CZ	2.35	0.56
1:A:144:ARG:NH1	1:A:148:ASP:OD1	2.39	0.56
2:D:95:LYS:HG3	2:D:96:PHE:N	2.21	0.56
1:B:52:ILE:HB	1:B:106:LEU:HB2	1.87	0.56
2:C:52:LEU:HD23	2:C:52:LEU:C	2.25	0.56
1:A:130:ARG:NH1	2:D:65:GLU:HG3	2.15	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LYS:O	1:B:63:LYS:HG3	2.05	0.56
2:C:55:LEU:HD22	2:C:78:SER:O	2.06	0.56
2:D:61:ASN:ND2	2:D:72:TYR:HE2	2.04	0.56
2:C:86:VAL:O	2:C:87:CYS:SG	2.64	0.56
1:A:83:PHE:CE1	1:A:112:VAL:HG22	2.41	0.56
1:B:35:THR:O	1:B:37(C):GLN:HA	2.06	0.55
2:D:80:ASN:HA	2:D:82:PHE:CE2	2.42	0.55
1:B:132:VAL:CG1	1:B:133:TYR:CZ	2.90	0.55
2:D:85:VAL:HG12	2:D:86:VAL:N	2.21	0.55
1:A:129:ASP:O	1:A:132:VAL:HG12	2.06	0.55
1:A:215:TRP:O	2:C:84:ARG:NH1	2.40	0.55
1:B:198(B):SER:HB2	1:B:203:TRP:CE3	2.42	0.55
1:A:44:ILE:O	1:A:121:PRO:HA	2.07	0.54
1:A:240:GLU:HG2	2:D:67:TRP:CH2	2.42	0.54
2:C:39:GLU:OE2	2:C:130:TRP:NE1	2.36	0.54
1:B:35:THR:HG22	1:B:65:LEU:HD23	1.88	0.54
2:C:129:VAL:HB	3:C:149:HOH:O	2.07	0.54
1:A:171:ARG:H	1:A:171:ARG:HD2	1.72	0.54
1:A:95:LYS:HD2	2:D:108:ARG:NE	2.21	0.54
1:B:189:ASP:CG	1:B:190:ALA:H	2.11	0.54
1:A:129:ASP:HB3	1:A:132:VAL:CG1	2.37	0.54
1:A:151:ILE:CG2	1:A:151:ILE:O	2.56	0.53
1:A:221:GLN:HB2	1:A:224:ARG:HB2	1.90	0.53
1:B:32:THR:HB	1:B:141:TRP:CZ3	2.44	0.53
1:A:116:ASP:HA	1:A:119:ARG:HH11	1.74	0.53
1:A:202(A):HIS:O	1:A:202(B):ASN:HB3	2.08	0.53
1:B:177:THR:N	1:B:180:MET:HE3	2.20	0.53
1:A:96:MET:CE	2:C:54:ARG:HD3	2.38	0.53
2:D:5:GLN:N	2:D:6:PRO:HD2	2.23	0.53
2:D:6:PRO:HG2	2:D:9:LYS:HB2	1.91	0.53
2:C:48:VAL:HB	2:C:52:LEU:HB3	1.91	0.53
1:A:161:PRO:HD3	1:A:184(A):TYR:CZ	2.44	0.53
1:B:38:HIS:HB3	1:B:151:ILE:HD12	1.91	0.53
1:A:222:ARG:HG3	1:A:222:ARG:NH1	2.18	0.52
2:C:37:LYS:HE2	2:D:130:TRP:CZ2	2.43	0.52
1:B:111:THR:CG2	1:B:112:VAL:N	2.72	0.52
1:B:51:TRP:CZ3	1:B:107:LYS:HB2	2.45	0.52
1:A:188(A):LYS:O	1:A:189:ASP:HB2	2.08	0.52
1:A:184(A):TYR:HE2	1:A:188(A):LYS:HD2	1.75	0.52
1:B:20:THR:O	1:B:157:LYS:HG2	2.10	0.52
2:D:30:GLN:HB2	2:D:33:GLU:HG2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:O	1:A:146:LEU:C	2.48	0.52
2:D:27:LEU:HD11	2:D:38:VAL:HG21	1.90	0.52
1:B:144:ARG:HD3	1:B:152:GLN:CD	2.30	0.51
1:A:163:VAL:CG2	1:A:182:CYS:HB2	2.40	0.51
1:A:123:CYS:O	1:A:204:HIS:HA	2.10	0.51
1:B:83:PHE:CZ	1:B:112:VAL:HG22	2.46	0.51
1:A:16:ILE:HD12	1:A:138:VAL:HG23	1.91	0.51
1:A:69:SER:HG	1:A:83:PHE:HE2	1.58	0.51
2:D:32:ASP:OD2	2:D:35:THR:HG23	2.11	0.51
1:A:63:LYS:HA	1:A:63:LYS:HE2	1.92	0.51
1:B:223:GLU:O	1:B:224:ARG:NH1	2.34	0.51
1:A:234:TYR:O	1:A:237:TRP:HB3	2.10	0.51
1:A:96:MET:SD	2:C:54:ARG:HD3	2.50	0.50
1:A:216:GLY:HA3	2:C:84:ARG:HH12	1.75	0.50
1:B:38:HIS:CE1	1:B:40:CYS:O	2.64	0.50
1:B:61:SER:HB3	1:B:64:ILE:CG2	2.41	0.50
2:D:140:VAL:CG1	2:D:141:VAL:N	2.75	0.50
1:B:32:THR:HG23	1:B:68:TYR:HB2	1.93	0.50
2:C:19:GLY:O	2:C:20:MET:CG	2.60	0.50
1:A:202(A):HIS:HE1	1:A:204:HIS:NE2	2.10	0.50
1:B:68:TYR:HB3	1:B:71:ILE:HG13	1.94	0.49
1:A:28:PRO:O	1:A:118:GLN:HA	2.12	0.49
1:A:57:HIS:ND1	1:A:102:ASP:OD2	2.46	0.49
1:A:202(B):ASN:O	1:A:202(C):GLU:HB2	2.13	0.49
1:B:145:LYS:O	1:B:149:ASP:HB2	2.13	0.49
1:B:149:ASP:CG	1:B:150:LYS:H	2.15	0.49
1:B:81:THR:HG22	1:B:81(A):SER:N	2.28	0.49
1:B:128:GLY:O	1:B:129:ASP:C	2.50	0.49
1:A:138:VAL:HG12	1:A:198(A):LEU:HD13	1.95	0.49
1:B:59:PHE:CZ	1:B:106:LEU:HD21	2.48	0.49
1:B:189:ASP:CG	1:B:190:ALA:N	2.66	0.49
2:C:27:LEU:HD11	2:C:38:VAL:HG21	1.95	0.49
1:B:75:ALA:C	1:B:77:ILE:N	2.64	0.48
1:B:143:TYR:HD1	1:B:143:TYR:N	2.10	0.48
1:B:171:ARG:HG2	1:B:223:GLU:O	2.13	0.48
1:A:222:ARG:HG2	1:A:223:GLU:HG3	1.95	0.48
1:A:223:GLU:O	1:A:224:ARG:HD3	2.14	0.48
1:A:144:ARG:NH1	1:A:152:GLN:CD	2.67	0.48
1:B:144:ARG:HD3	1:B:152:GLN:NE2	2.28	0.48
1:A:91:HIS:HD2	1:A:93:GLN:HB2	1.78	0.48
1:B:178:HIS:CE1	1:B:179:LYS:HZ2	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:HD22	1:A:233:GLU:CG	2.26	0.48
2:D:7:LEU:HG	2:D:13:TYR:CD2	2.49	0.48
2:C:54:ARG:NE	2:C:100:TYR:HB2	2.29	0.48
1:A:230:ASN:HD22	1:A:233:GLU:HG2	1.79	0.48
1:A:36:THR:HG23	1:A:66:ARG:HD3	1.96	0.48
1:B:132:VAL:O	1:B:132:VAL:HG13	2.13	0.48
1:B:34:HIS:O	1:B:65:LEU:HA	2.13	0.48
2:D:36:LEU:O	2:D:37:LYS:HG3	2.12	0.48
1:B:176:ILE:CA	1:B:180:MET:HE3	2.43	0.48
1:A:190:ALA:HB1	1:A:194:ASP:CB	2.43	0.48
1:A:173:ARG:HG2	2:C:76:LYS:CE	2.44	0.48
1:A:91:HIS:CD2	1:A:93:GLN:HB2	2.49	0.48
1:B:143:TYR:CD1	1:B:143:TYR:N	2.81	0.48
2:D:74:PHE:HZ	2:D:99:ALA:CB	2.27	0.48
1:A:33:LEU:O	1:A:39:LEU:HB3	2.14	0.47
2:C:21:LYS:HE2	2:C:121:ASP:O	2.14	0.47
2:C:51:ASN:HB3	2:C:82:PHE:CB	2.36	0.47
1:A:57:HIS:NE2	2:C:85:VAL:HG23	2.29	0.47
1:B:130:ARG:HH21	2:C:65:GLU:CG	2.27	0.47
2:D:64:LEU:O	2:D:67:TRP:HB2	2.14	0.47
2:D:86:VAL:O	2:D:87:CYS:SG	2.72	0.47
1:B:181:ILE:HG23	1:B:228:TYR:HB2	1.95	0.47
1:A:16:ILE:HB	1:A:156:GLN:CB	2.39	0.47
1:A:173:ARG:O	1:A:173:ARG:HG3	2.15	0.47
1:B:30:GLN:HG2	1:B:155:LEU:HD21	1.95	0.47
1:A:169:GLN:NE2	1:A:174:HIS:O	2.44	0.47
1:A:20:THR:HG22	1:A:21:ALA:N	2.28	0.47
1:A:32:THR:CG2	1:A:68:TYR:HB2	2.45	0.47
1:B:35:THR:HG22	1:B:65:LEU:CD2	2.44	0.47
1:A:149:LYS:O	1:A:151:ILE:C	2.52	0.47
2:D:74:PHE:HB2	2:D:119:THR:HG22	1.96	0.47
1:A:83:PHE:CZ	1:A:112:VAL:HG22	2.49	0.47
1:A:16:ILE:CB	1:A:156:GLN:HB3	2.39	0.47
1:B:63:LYS:HB2	1:B:63:LYS:HE3	1.68	0.47
1:B:115:ALA:O	1:B:119:ARG:HG3	2.14	0.47
2:C:48:VAL:HG11	2:C:97:VAL:HG11	1.97	0.47
1:A:27:TRP:N	1:A:28:PRO:CD	2.77	0.47
1:A:90:ILE:HG12	1:A:104:ALA:CB	2.45	0.46
1:A:195:SER:C	1:A:197:GLY:H	2.17	0.46
1:A:140:GLY:HA3	1:A:194:ASP:OD1	2.16	0.46
2:C:126:LYS:HE2	2:D:138:ASN:OD1	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:LYS:HB2	2:D:71:TYR:CE1	2.50	0.46
2:C:72:TYR:CD1	2:C:72:TYR:N	2.84	0.46
1:B:72:LEU:HD12	1:B:72:LEU:O	2.15	0.46
2:C:103:ASP:CB	2:D:103:ASP:HB3	2.34	0.46
1:B:44:ILE:HG22	1:B:121:PRO:HB3	1.98	0.46
1:A:173(A):GLY:HA3	3:C:143:HOH:O	2.14	0.46
1:A:23:VAL:HG22	1:A:24:ARG:H	1.79	0.46
1:A:202(A):HIS:ND1	1:A:202(A):HIS:O	2.49	0.46
1:A:185:ARG:HH12	1:A:222:ARG:NH2	2.14	0.46
1:A:56:ALA:N	1:A:102:ASP:OD1	2.49	0.46
2:C:52:LEU:HD23	2:C:53:HIS:N	2.31	0.46
1:B:192:LYS:HA	2:D:84:ARG:CA	2.46	0.46
1:B:57:HIS:CE1	1:B:102:ASP:OD1	2.69	0.46
1:B:64:ILE:HG13	1:B:64:ILE:O	2.15	0.45
2:C:64:LEU:HB3	2:C:67:TRP:HB2	1.98	0.45
1:B:75:ALA:O	1:B:76:GLU:C	2.55	0.45
1:B:32:THR:CG2	1:B:68:TYR:HB2	2.47	0.45
2:C:95:LYS:HG2	2:C:96:PHE:N	2.31	0.45
1:B:198(B):SER:HB2	1:B:203:TRP:HE3	1.81	0.45
2:D:19:GLY:HA2	2:D:121:ASP:OD2	2.16	0.45
2:D:23:GLN:NE2	2:D:125:VAL:HG23	2.31	0.45
2:C:129:VAL:CG1	2:C:130:TRP:N	2.79	0.45
1:A:169:GLN:NE2	1:A:169:GLN:HA	2.31	0.45
1:A:89:ILE:O	1:A:104:ALA:HB1	2.17	0.45
1:A:186:GLU:CD	1:A:186:GLU:H	2.20	0.45
1:B:192:LYS:HA	2:D:84:ARG:HA	1.97	0.45
2:D:27:LEU:HB3	2:D:109:TYR:CZ	2.52	0.45
2:D:74:PHE:CB	2:D:119:THR:HG22	2.46	0.45
2:C:64:LEU:HA	2:C:64:LEU:HD12	1.80	0.44
1:A:145:LYS:O	1:A:145:LYS:CG	2.66	0.44
1:A:20:THR:CG2	1:A:21:ALA:N	2.81	0.44
1:B:131:ASN:OD1	1:B:131:ASN:O	2.35	0.44
2:C:57:GLY:HA2	2:C:76:LYS:O	2.18	0.44
1:A:86:GLN:HB3	1:A:107:LYS:O	2.17	0.44
1:A:138:VAL:CG2	1:A:138:VAL:O	2.65	0.44
1:B:181:ILE:CG2	1:B:228:TYR:HB2	2.47	0.44
2:C:18:LYS:CG	2:C:18:LYS:O	2.64	0.44
1:B:89:ILE:HB	1:B:105:LEU:HB2	1.98	0.44
1:A:138:VAL:HG12	1:A:198(A):LEU:HD12	1.99	0.44
1:B:111:THR:HG22	1:B:112:VAL:H	1.83	0.44
1:A:37(D):ARG:NH2	2:C:88:PRO:CD	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:THR:OG1	1:B:38:HIS:ND1	2.44	0.44
2:D:17:GLU:O	2:D:18:LYS:C	2.55	0.44
2:D:80:ASN:ND2	2:D:80:ASN:O	2.50	0.44
1:A:36:THR:CG2	1:A:66:ARG:HD3	2.48	0.43
2:C:37:LYS:HG3	2:D:130:TRP:CZ3	2.53	0.43
1:B:29:TRP:HB3	1:B:119:ARG:O	2.18	0.43
1:B:45:ILE:HD13	1:B:53:LEU:HB2	1.99	0.43
2:D:134:GLU:O	2:D:135:LYS:C	2.56	0.43
1:B:217:GLU:HG2	1:B:221:GLN:HE21	1.82	0.43
1:A:61:SER:O	1:A:64:ILE:HG12	2.17	0.43
1:A:181:ILE:HG23	1:A:228:TYR:HB2	2.00	0.43
1:B:32:THR:O	1:B:32:THR:HG23	2.18	0.43
1:B:113:ASN:O	1:B:118:GLN:NE2	2.51	0.43
1:B:179:LYS:HE3	2:C:68:GLY:HA2	2.01	0.43
1:B:234:TYR:O	1:B:235:VAL:C	2.55	0.43
1:A:195:SER:OG	2:C:84:ARG:C	2.57	0.43
1:B:202(B):ASN:O	1:B:202(D):VAL:HG23	2.17	0.43
1:B:236:ASP:HB2	2:C:66:GLY:O	2.18	0.43
1:A:237:TRP:HB2	2:D:67:TRP:HA	2.00	0.43
1:A:116:ASP:OD2	1:A:119:ARG:NH1	2.52	0.43
2:C:80:ASN:HA	2:C:82:PHE:CE1	2.54	0.43
1:B:221:GLN:HB2	1:B:224:ARG:HB2	2.00	0.43
1:A:144:ARG:HH11	1:A:144:ARG:CG	2.28	0.43
1:A:202(A):HIS:CE1	1:A:204:HIS:NE2	2.87	0.43
1:A:96:MET:HE3	2:C:53:HIS:HB2	2.01	0.42
1:A:43:SER:O	1:A:52:ILE:HA	2.19	0.42
1:A:29:TRP:NE1	1:A:122:ILE:HD12	2.34	0.42
2:D:64:LEU:HD12	2:D:64:LEU:HA	1.80	0.42
2:D:85:VAL:CG1	2:D:86:VAL:N	2.81	0.42
1:A:181:ILE:CG2	1:A:228:TYR:HB2	2.49	0.42
1:A:223:GLU:O	1:A:224:ARG:CD	2.68	0.42
1:B:37(A):PRO:HG2	1:B:37(B):THR:H	1.83	0.42
1:B:230:ASN:ND2	1:B:233:GLU:HG2	2.34	0.42
1:A:202(A):HIS:HE1	1:A:204:HIS:CE1	2.38	0.42
2:C:33:GLU:HG2	2:C:109:TYR:CD1	2.55	0.42
2:C:135:LYS:O	2:C:136:ILE:HG12	2.19	0.42
1:A:173:ARG:HG2	2:C:76:LYS:CD	2.50	0.42
1:B:65:LEU:C	1:B:66:ARG:HG2	2.40	0.42
1:A:143:TYR:HD2	1:A:146:LEU:O	2.03	0.42
1:A:78:LYS:N	1:A:81:THR:OG1	2.47	0.42
2:D:6:PRO:HG2	2:D:9:LYS:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:THR:CG2	1:B:112:VAL:H	2.33	0.42
2:C:129:VAL:HG12	2:C:130:TRP:N	2.35	0.42
1:A:154:THR:O	1:A:155:LEU:C	2.58	0.42
1:B:47:ASN:HB2	1:B:111:THR:HG23	2.02	0.42
1:B:96:MET:HE2	2:D:54:ARG:NE	2.34	0.41
2:C:18:LYS:HG2	2:C:18:LYS:O	2.20	0.41
1:A:129:ASP:C	1:A:132:VAL:HG12	2.41	0.41
1:A:210:VAL:HG13	3:A:263:HOH:O	2.19	0.41
1:B:181:ILE:O	1:B:228:TYR:N	2.40	0.41
2:C:138:ASN:OD1	2:D:126:LYS:HG2	2.19	0.41
2:C:42:ILE:HD12	2:C:101:LEU:CD1	2.46	0.41
1:B:38:HIS:HB2	1:B:74:GLN:OE1	2.19	0.41
1:A:141:TRP:CZ2	1:A:155:LEU:HD13	2.55	0.41
2:C:42:ILE:HG12	2:C:125:VAL:HG22	2.02	0.41
1:A:202:LYS:HB2	1:A:203:TRP:CH2	2.55	0.41
1:A:34:HIS:CE1	1:A:74:GLN:OE1	2.74	0.41
1:B:17:VAL:O	1:B:188(A):LYS:HA	2.20	0.41
2:D:19:GLY:C	2:D:121:ASP:OD2	2.59	0.41
1:A:137:TRP:CZ2	1:A:159:LYS:HD2	2.55	0.41
1:A:135:ASP:OD1	1:A:159:LYS:HE3	2.19	0.41
1:A:125:PRO:HB2	1:A:232:VAL:HG22	2.02	0.41
1:B:143:TYR:H	1:B:143:TYR:HD1	1.68	0.41
2:C:12:PRO:HD2	2:C:64:LEU:HD21	2.02	0.41
1:B:96:MET:HE3	2:D:53:HIS:HB2	2.02	0.41
2:C:8:GLU:O	2:C:11:ALA:N	2.54	0.41
1:A:144:ARG:HH11	1:A:152:GLN:CD	2.24	0.41
1:A:222:ARG:O	1:A:223:GLU:HB2	2.21	0.41
2:C:11:ALA:O	2:C:13:TYR:N	2.49	0.41
1:A:82:PHE:C	1:A:82:PHE:CD1	2.94	0.41
1:B:188(A):LYS:O	1:B:189:ASP:HB2	2.20	0.41
2:C:69:TYR:N	2:C:69:TYR:CD1	2.88	0.41
2:C:135:LYS:C	2:C:136:ILE:HG12	2.40	0.41
2:C:85:VAL:CG1	2:C:86:VAL:N	2.84	0.41
2:C:122:ASN:ND2	2:C:122:ASN:H	2.19	0.41
2:D:44:GLN:HG2	2:D:55:LEU:HD11	2.02	0.41
1:A:27:TRP:C	1:A:29:TRP:H	2.24	0.40
2:C:55:LEU:CD2	2:C:79:SER:HA	2.50	0.40
1:A:222:ARG:NH1	1:A:222:ARG:CG	2.82	0.40
2:D:64:LEU:HB3	2:D:67:TRP:HB2	2.03	0.40
2:C:20:MET:N	2:C:121:ASP:OD1	2.53	0.40
2:C:55:LEU:HD22	2:C:79:SER:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:N	1:A:80:ASP:OD1	2.54	0.40
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.87	0.40
1:A:144:ARG:CG	1:A:144:ARG:NH1	2.83	0.40
2:D:32:ASP:HA	3:D:150:HOH:O	2.21	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	236/238 (99%)	202 (86%)	28 (12%)	6 (2%)	7 26
1	B	236/238 (99%)	199 (84%)	30 (13%)	7 (3%)	5 21
2	C	135/142 (95%)	113 (84%)	19 (14%)	3 (2%)	8 30
2	D	130/142 (92%)	112 (86%)	14 (11%)	4 (3%)	5 20
All	All	737/760 (97%)	626 (85%)	91 (12%)	20 (3%)	6 24

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	LEU
1	B	128	GLY
1	B	129	ASP
1	B	222	ARG
2	C	18	LYS
2	D	135	LYS
1	A	185	ARG
1	B	59(A)	TYR
1	B	76	GLU
1	A	37(A)	PRO
1	A	151	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	139	ALA
1	A	76	GLU
2	D	18	LYS
2	D	65	GLU
2	D	134	GLU
2	C	14	PRO
1	B	235	VAL
1	B	132	VAL
1	A	27	TRP

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	202/202 (100%)	192 (95%)	10 (5%)	30 65
1	B	202/202 (100%)	180 (89%)	22 (11%)	8 23
2	C	122/126 (97%)	111 (91%)	11 (9%)	12 34
2	D	120/126 (95%)	108 (90%)	12 (10%)	9 28
All	All	646/656 (98%)	591 (92%)	55 (8%)	13 36

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	34	HIS
1	A	80	ASP
1	A	132	VAL
1	A	147	ARG
1	A	151	ILE
1	A	156	GLN
1	A	171	ARG
1	A	186	GLU
1	A	202(A)	HIS
1	B	17	VAL
1	B	30	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	LEU
1	B	37	SER
1	B	43	SER
1	B	60	GLU
1	B	63	LYS
1	B	66	ARG
1	B	79	GLU
1	B	93	GLN
1	B	98	GLU
1	B	110	THR
1	B	117	SER
1	B	130	ARG
1	B	131	ASN
1	B	144	ARG
1	B	151	ILE
1	B	171	ARG
1	B	173	ARG
1	B	198(B)	SER
1	B	222	ARG
1	B	245	VAL
2	C	17	GLU
2	C	23	GLN
2	C	26	GLN
2	C	60	GLU
2	C	79	SER
2	C	80	ASN
2	C	82	PHE
2	C	84	ARG
2	C	86	VAL
2	C	91	LYS
2	C	122	ASN
2	D	15	GLN
2	D	47	GLU
2	D	53	HIS
2	D	54	ARG
2	D	58	LYS
2	D	61	ASN
2	D	75	ASP
2	D	76	LYS
2	D	82	PHE
2	D	84	ARG
2	D	93	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	137	ASP

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	30	GLN
1	A	34	HIS
1	A	37(C)	GLN
1	A	48	GLN
1	A	73	ASN
1	A	86	GLN
1	A	91	HIS
1	A	93	GLN
1	A	118	GLN
1	A	152	GLN
1	A	156	GLN
1	A	202(A)	HIS
1	A	204	HIS
1	A	221	GLN
1	A	230	ASN
1	A	243	GLN
1	B	30	GLN
1	B	37(C)	GLN
1	B	48	GLN
1	B	86	GLN
1	B	118	GLN
1	B	156	GLN
1	B	178	HIS
1	B	202(B)	ASN
1	B	221	GLN
2	C	23	GLN
2	C	51	ASN
2	C	80	ASN
2	C	122	ASN
2	D	15	GLN
2	D	51	ASN
2	D	61	ASN
2	D	80	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	238/238 (100%)	-0.24	1 (0%)	93	92	19, 35, 55, 65	0
1	B	238/238 (100%)	-0.10	3 (1%)	79	78	26, 40, 64, 82	0
2	C	137/142 (96%)	0.01	4 (2%)	55	49	25, 44, 72, 79	0
2	D	134/142 (94%)	-0.14	1 (0%)	89	88	22, 41, 57, 69	0
All	All	747/760 (98%)	-0.13	9 (1%)	81	78	19, 39, 62, 82	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	GLY	3.8
2	C	88	PRO	3.7
1	A	245	VAL	3.6
2	C	86	VAL	3.2
2	C	89	ASP	2.9
2	C	87	CYS	2.8
1	B	127	LYS	2.1
1	B	245	VAL	2.1
2	D	18	LYS	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.