Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:51 PM GMT

PDB ID	:	1HIA
Title	:	KALLIKREIN COMPLEXED WITH HIRUSTASIN
Authors	:	Mittl, P.; Di Marco, S.; Gruetter, M.
Deposited on	:	1996-12-12
Resolution	:	2.40 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:

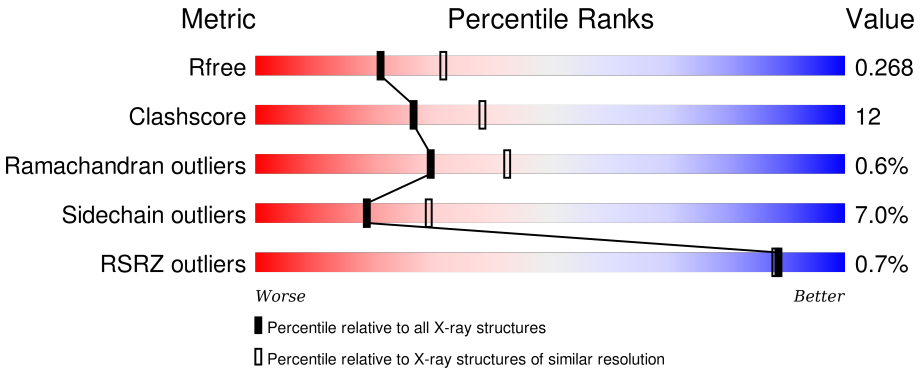
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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.



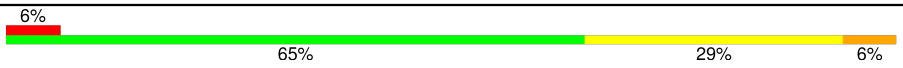
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	80	68% 28% 5%
1	X	80	% 75% 24% .
2	B	152	82% 16% ..
2	Y	152	72% 25% ..
3	I	48	73% 17% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	J	48	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4584 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 KALLIKREIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	80	Total	C	N	O	S	0	0	0
			646	414	113	116	3			
1	X	80	Total	C	N	O	S	0	0	0
			646	414	113	116	3			

- Molecule 2 is a protein called KALLIKREIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1141	719	180	231	11			
2	Y	150	Total	C	N	O	S	0	0	0
			1141	719	180	231	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	ASP	-	INSERTION	UNP P00752
B	170	ASP	-	INSERTION	UNP P00752
B	174	ASP	-	INSERTION	UNP P00752
B	239	ASP	ASN	CONFLICT	UNP P00752
Y	148	ASP	-	INSERTION	UNP P00752
Y	170	ASP	-	INSERTION	UNP P00752
Y	174	ASP	-	INSERTION	UNP P00752
Y	239	ASP	ASN	CONFLICT	UNP P00752

- Molecule 3 is a protein called HIRUSTASIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	48	Total	C	N	O	S	0	0	0
			353	210	65	68	10			
3	J	48	Total	C	N	O	S	0	0	0
			353	210	65	68	10			

- Molecule 4 is water.

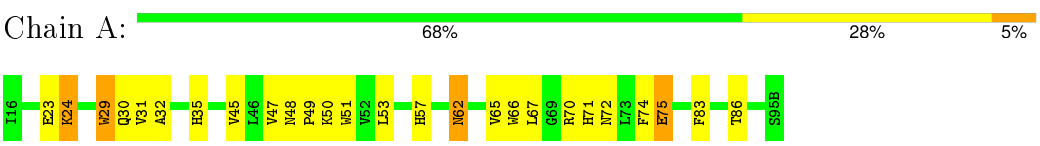
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	42	Total O 42 42	0	0
4	B	101	Total O 101 101	0	0
4	I	20	Total O 20 20	0	0
4	J	10	Total O 10 10	0	0
4	X	44	Total O 44 44	0	0
4	Y	87	Total O 87 87	0	0

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.

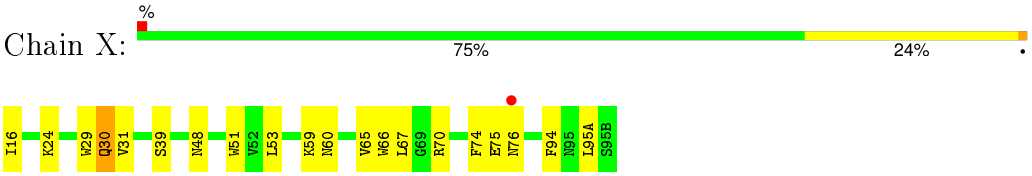
- Molecule 1: KALLIKREIN

Chain A:



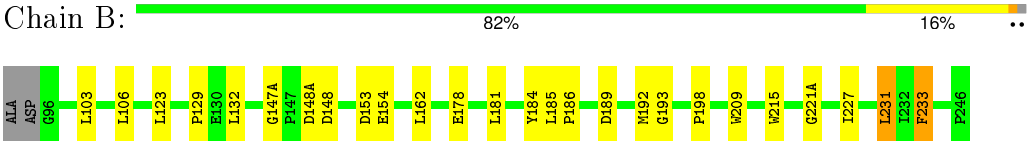
- Molecule 1: KALLIKREIN

Chain X:



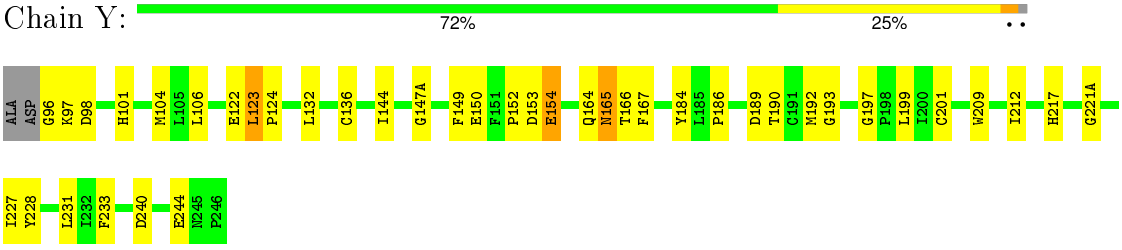
- Molecule 2: KALLIKREIN

Chain B:



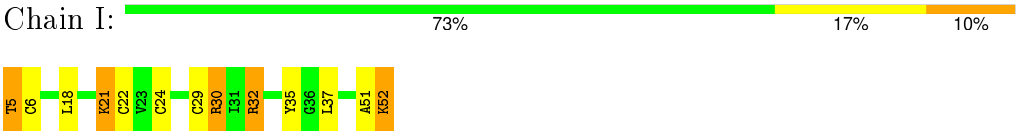
- Molecule 2: KALLIKREIN

Chain Y:



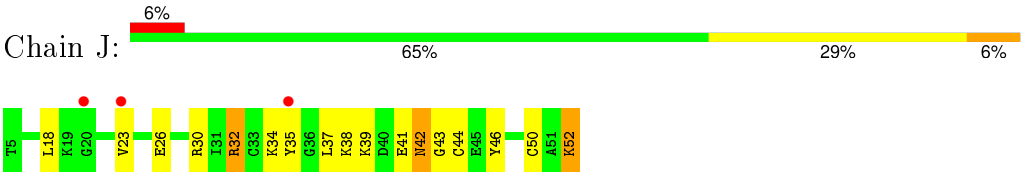
- Molecule 3: HIRUSTASIN

Chain I:



- Molecule 3: HIRUSTASIN

Chain J:


6%
65%
29%
6%
T5
L18
K19
G20
V23
E26
R30
Y31
R32
C33
K34
Y35
G36
L37
K38
K39
D40
E41
M42
G43
C44
E45
Y46
C50
A51
K52

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.90Å 86.00Å 69.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.9 (8.00-2.40) 89.3 (8.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.40Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.205 , 0.311 0.175 , 0.268	Depositor DCC
R_{free} test set	2435 reflections (10.03%)	DCC
Wilson B-factor (Å^2)	39.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.12 , 56.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.30$	Xtriage
Outliers	6 of 26769 reflections (0.022%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4584	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 47.94 % 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 9.2307e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.63	0/669	0.80	0/910
1	X	0.58	0/669	0.78	0/910
2	B	0.54	0/1171	0.81	0/1596
2	Y	0.52	0/1171	0.78	0/1596
3	I	0.49	0/356	0.72	0/472
3	J	0.41	0/356	0.71	0/472
All	All	0.54	0/4392	0.78	0/5956

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	646	0	589	23	0
1	X	646	0	589	17	0
2	B	1141	0	1076	21	0
2	Y	1141	0	1076	32	0
3	I	353	0	337	14	0
3	J	353	0	337	15	0
4	A	42	0	0	1	0
4	B	101	0	0	2	0
4	I	20	0	0	2	0
4	J	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	X	44	0	0	0	0
4	Y	87	0	0	4	0
All	All	4584	0	4004	100	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 12.

All (100) 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:X:75:GLU:HG2	1:X:76:ASN:H	1.47	0.79
2:B:178:GLU:HG3	2:Y:144:ILE:CD1	2.23	0.69
2:Y:199:LEU:HD22	2:Y:228:TYR:CG	2.28	0.68
2:Y:209:TRP:CE2	2:Y:231:LEU:HD11	2.32	0.65
1:A:48:ASN:HD22	1:A:50:LYS:H	1.42	0.65
3:I:21:LYS:HE3	3:I:21:LYS:HA	1.80	0.64
3:J:18:LEU:HB2	3:J:23:VAL:HG11	1.79	0.64
3:I:21:LYS:HE3	3:I:22:CYS:H	1.64	0.63
1:A:48:ASN:ND2	1:A:50:LYS:H	1.98	0.61
1:A:35:HIS:HD2	1:A:62:ASN:O	1.84	0.61
1:X:39:SER:HB2	3:J:34:LYS:HE2	1.83	0.60
2:B:178:GLU:HG3	2:Y:144:ILE:HD12	1.85	0.59
1:A:70:ARG:NH2	1:A:75:GLU:O	2.34	0.59
1:A:24:LYS:HE2	1:A:24:LYS:H	1.66	0.58
1:A:32:ALA:HB3	1:A:66:TRP:HB2	1.84	0.57
3:J:39:LYS:HE3	3:J:43:GLY:O	2.05	0.57
1:X:94:PHE:HB2	2:Y:101:HIS:O	2.03	0.57
3:J:52:LYS:HZ3	3:J:52:LYS:HB2	1.70	0.56
2:Y:152:PRO:HA	4:Y:282:HOH:O	2.06	0.56
2:Y:123:LEU:HB2	4:Y:288:HOH:O	2.06	0.55
2:Y:192:MET:HE1	3:J:37:LEU:HD11	1.88	0.55
1:X:16:ILE:HD13	2:Y:190:THR:HA	1.89	0.55
2:Y:197:GLY:O	2:Y:212:ILE:HA	2.08	0.54
3:I:35:TYR:HB2	3:I:51:ALA:HB3	1.88	0.54
3:J:41:GLU:HG3	3:J:42:ASN:OD1	2.07	0.54
3:I:6:CYS:HB3	3:I:22:CYS:SG	2.47	0.53
1:A:29:TRP:CZ3	2:B:198:PRO:HG3	2.43	0.53
1:X:53:LEU:HD12	2:Y:104:MET:O	2.09	0.53
3:J:52:LYS:NZ	3:J:52:LYS:HB2	2.24	0.53
1:A:48:ASN:HB3	1:A:51:TRP:HB2	1.92	0.52
2:Y:193:GLY:HA2	3:J:32:ARG:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:18:LEU:HB2	3:J:23:VAL:CG1	2.39	0.52
1:A:24:LYS:HD3	1:A:71:HIS:CE1	2.45	0.51
1:A:45:VAL:HG22	2:B:198:PRO:HD3	1.92	0.51
2:Y:184:TYR:CE2	2:Y:186:PRO:HB2	2.47	0.50
2:Y:136:CYS:HA	2:Y:201:CYS:HA	1.92	0.50
1:A:31:VAL:HG22	1:A:67:LEU:HD23	1.94	0.50
1:A:24:LYS:HD2	4:A:127:HOH:O	2.11	0.49
2:B:162:LEU:HD11	2:B:181:LEU:HD22	1.94	0.49
1:A:74:PHE:CD2	2:B:153:ASP:HA	2.48	0.48
2:B:129:PRO:HB2	2:B:162:LEU:CD2	2.43	0.48
1:X:66:TRP:HB3	1:X:70:ARG:HD2	1.95	0.48
1:X:75:GLU:HG2	1:X:76:ASN:N	2.24	0.48
1:X:59:LYS:HB3	2:Y:104:MET:SD	2.54	0.48
1:A:31:VAL:HG22	1:A:67:LEU:CD2	2.44	0.48
3:I:29:CYS:HB3	4:I:54:HOH:O	2.13	0.48
1:A:31:VAL:CG1	1:A:65:VAL:HG13	2.44	0.47
2:B:209:TRP:CZ2	2:B:231:LEU:HD11	2.48	0.47
2:B:233:PHE:HZ	2:Y:144:ILE:HD12	1.79	0.47
2:Y:167:PHE:HE2	4:Y:263:HOH:O	1.97	0.47
1:A:53:LEU:HD11	2:B:103:LEU:HD12	1.96	0.47
3:I:30:ARG:N	3:I:30:ARG:HD2	2.29	0.47
2:Y:240:ASP:O	2:Y:244:GLU:HG2	2.15	0.46
1:X:31:VAL:HG22	1:X:67:LEU:CD2	2.45	0.46
2:B:184:TYR:CE2	2:B:186:PRO:HB2	2.51	0.46
1:X:74:PHE:HD2	2:Y:153:ASP:OD1	1.99	0.46
2:Y:227:ILE:HD12	2:Y:227:ILE:N	2.31	0.46
2:B:123:LEU:HD23	2:B:209:TRP:CZ3	2.51	0.46
2:Y:209:TRP:CZ2	2:Y:231:LEU:HD11	2.51	0.45
1:X:31:VAL:CG1	1:X:65:VAL:HG13	2.46	0.45
2:B:215:TRP:CZ2	2:B:227:ILE:HG13	2.52	0.45
2:Y:144:ILE:HG12	2:Y:150:GLU:O	2.17	0.45
3:J:39:LYS:HA	3:J:44:CYS:O	2.16	0.45
3:I:52:LYS:NZ	3:I:52:LYS:HB2	2.32	0.45
2:B:147(A):GLY:HA2	2:B:148:ASP:O	2.16	0.45
2:B:178:GLU:H	2:B:178:GLU:CD	2.21	0.44
1:X:59:LYS:HB2	1:X:59:LYS:HE3	1.42	0.44
2:B:132:LEU:HG	4:B:339:HOH:O	2.18	0.44
1:A:86:THR:HG21	4:B:287:HOH:O	2.17	0.44
3:J:50:CYS:O	3:J:52:LYS:HD3	2.17	0.44
2:Y:147(A):GLY:HA3	2:Y:149:PHE:CE1	2.52	0.44
3:I:5:THR:HB	3:I:6:CYS:H	1.59	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:96:GLY:O	2:Y:97:LYS:HD3	2.18	0.44
1:A:57:HIS:CE1	3:I:29:CYS:HB2	2.53	0.43
3:J:41:GLU:HG3	3:J:42:ASN:H	1.83	0.43
2:B:192:MET:CE	3:I:37:LEU:HD21	2.49	0.43
3:I:35:TYR:HD2	3:I:51:ALA:O	2.00	0.43
1:A:67:LEU:HD12	1:A:83:PHE:CE2	2.54	0.43
2:Y:189:ASP:HB2	2:Y:221(A):GLY:HA2	2.00	0.43
3:J:37:LEU:HD23	3:J:46:TYR:O	2.19	0.43
1:X:30:GLN:HE21	1:X:30:GLN:HB2	1.67	0.42
1:A:72:ASN:OD1	2:B:153:ASP:HB3	2.19	0.42
2:Y:154:GLU:H	2:Y:154:GLU:CD	2.22	0.42
2:Y:124:PRO:HB3	2:Y:209:TRP:O	2.20	0.41
2:Y:165:ASN:ND2	4:Y:252:HOH:O	2.53	0.41
3:J:38:LYS:O	3:J:46:TYR:HD1	2.02	0.41
1:A:31:VAL:HG13	1:A:65:VAL:HG13	2.02	0.41
2:Y:217:HIS:CD2	3:J:26:GLU:HB3	2.55	0.41
2:B:189:ASP:HB2	2:B:221(A):GLY:HA2	2.02	0.41
1:X:74:PHE:CD2	2:Y:153:ASP:OD1	2.74	0.41
3:I:18:LEU:N	3:I:21:LYS:O	2.54	0.41
1:A:74:PHE:HD2	2:B:153:ASP:HA	1.85	0.41
1:A:47:VAL:HG11	1:A:53:LEU:HB2	2.03	0.41
1:X:30:GLN:HG3	1:X:31:VAL:N	2.35	0.41
2:B:193:GLY:HA2	3:I:32:ARG:HB2	2.03	0.41
1:X:48:ASN:HB3	1:X:51:TRP:HB2	2.03	0.40
3:I:24:CYS:HB2	4:I:69:HOH:O	2.21	0.40
2:Y:132:LEU:HA	2:Y:132:LEU:HD23	1.96	0.40
2:Y:122:GLU:CD	2:Y:122:GLU:H	2.23	0.40
1:X:31:VAL:HG22	1:X:67:LEU:HD21	2.03	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	78/80 (98%)	72 (92%)	5 (6%)	1 (1%)	15 21
1	X	78/80 (98%)	71 (91%)	6 (8%)	1 (1%)	15 21
2	B	148/152 (97%)	143 (97%)	5 (3%)	0	100 100
2	Y	148/152 (97%)	136 (92%)	11 (7%)	1 (1%)	26 38
3	I	46/48 (96%)	42 (91%)	4 (9%)	0	100 100
3	J	46/48 (96%)	35 (76%)	11 (24%)	0	100 100
All	All	544/560 (97%)	499 (92%)	42 (8%)	3 (1%)	30 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	24	LYS
1	A	75	GLU
2	Y	98	ASP

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	68/68 (100%)	62 (91%)	6 (9%)	12 18
1	X	68/68 (100%)	64 (94%)	4 (6%)	24 38
2	B	128/129 (99%)	122 (95%)	6 (5%)	32 50
2	Y	128/129 (99%)	121 (94%)	7 (6%)	27 42
3	I	40/40 (100%)	35 (88%)	5 (12%)	6 7
3	J	40/40 (100%)	35 (88%)	5 (12%)	6 7
All	All	472/474 (100%)	439 (93%)	33 (7%)	19 29

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

Mol	Chain	Res	Type
1	A	23	GLU
1	A	24	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	29	TRP
1	A	30	GLN
1	A	49	PRO
1	A	62	ASN
2	B	106	LEU
2	B	148(A)	ASP
2	B	154	GLU
2	B	185	LEU
2	B	231	LEU
2	B	233	PHE
3	I	5	THR
3	I	21	LYS
3	I	30	ARG
3	I	32	ARG
3	I	52	LYS
1	X	29	TRP
1	X	30	GLN
1	X	60	ASN
1	X	95(A)	LEU
2	Y	106	LEU
2	Y	123	LEU
2	Y	154	GLU
2	Y	164	GLN
2	Y	165	ASN
2	Y	166	THR
2	Y	233	PHE
3	J	30	ARG
3	J	32	ARG
3	J	35	TYR
3	J	42	ASN
3	J	52	LYS

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	30	GLN
1	A	48	ASN
1	A	62	ASN
2	B	165	ASN
1	X	30	GLN
1	X	48	ASN
1	X	60	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Y	109	GLN
2	Y	156	GLN
2	Y	165	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	80/80 (100%)	-0.96	0 100 100	21, 33, 80, 106	0
1	X	80/80 (100%)	-0.78	1 (1%) 79 79	20, 38, 84, 115	0
2	B	150/152 (98%)	-1.10	0 100 100	21, 33, 58, 87	0
2	Y	150/152 (98%)	-0.97	0 100 100	22, 36, 63, 93	0
3	I	48/48 (100%)	-0.34	0 100 100	28, 58, 96, 111	0
3	J	48/48 (100%)	0.41	3 (6%) 23 24	34, 84, 127, 133	0
All	All	556/560 (99%)	-0.80	4 (0%) 89 88	20, 37, 97, 133	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	20	GLY	5.3
3	J	35	TYR	3.2
3	J	23	VAL	3.0
1	X	76	ASN	2.4

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 (i)

There are no such residues in this entry.