Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:29 PM GMT

PDB ID	:	1KIG
Title	:	BOVINE FACTOR XA
Authors	:	Wei, A.; Alexander, R.; Chang, C.-H.
Deposited on	:	1997-04-24
Resolution	:	3.00 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 ⓘ symbol.

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

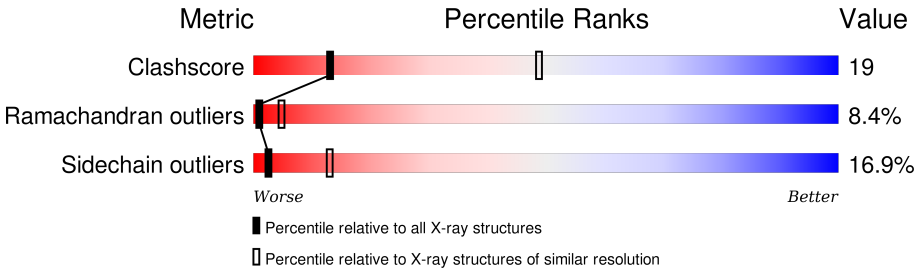
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.00 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	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	241	39% 49% 11%
2	L	51	41% 47% 10%
3	I	60	28% 43% 23% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2756 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 FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	20	0	0
			1880	1179	332	354	15			

- Molecule 2 is a protein called FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	51	Total	C	N	O	S	14	0	0
			388	228	73	80	7			

- Molecule 3 is a protein called ANTICOAGULANT PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	60	Total	C	N	O	S	0	0	0
			488	301	85	96	6			

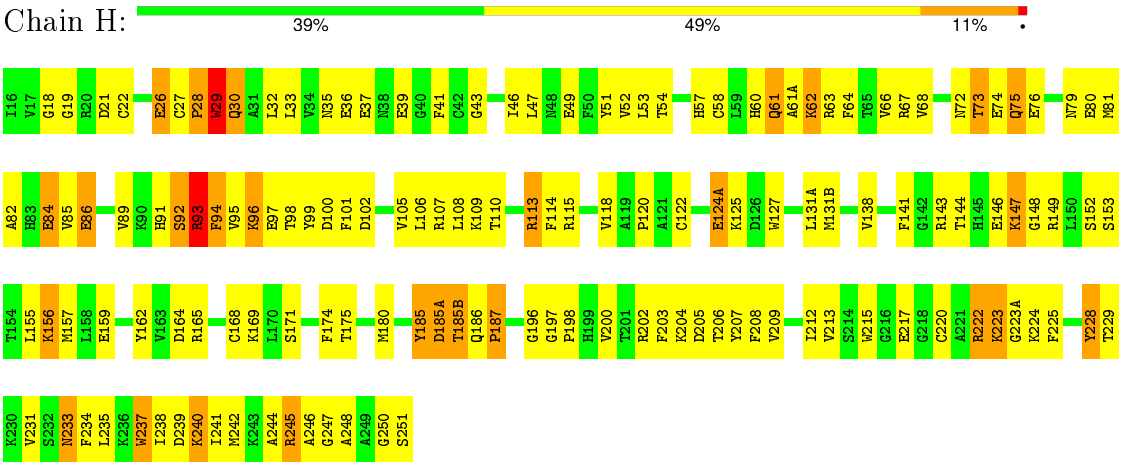
3 Residue-property plots (i)

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.

Note EDS was not executed.

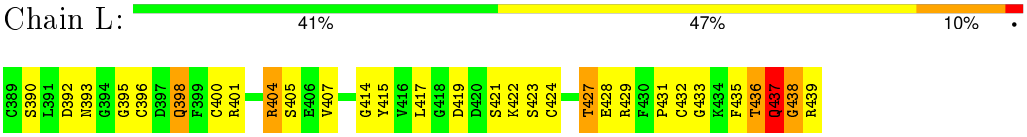
- Molecule 1: FACTOR XA

Chain H:



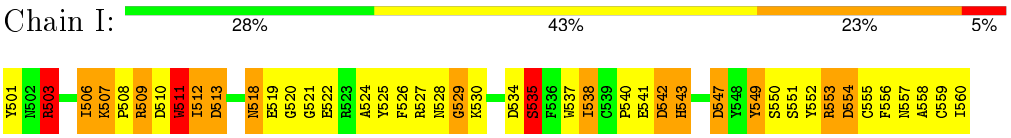
- Molecule 2: FACTOR XA

Chain L:



- Molecule 3: ANTICOAGULANT PEPTIDE

Chain I:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.10Å 133.10Å 68.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2756	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

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	H	0.97	0/1920	1.89	52/2588 (2.0%)
2	L	1.02	0/393	1.89	9/522 (1.7%)
3	I	1.11	0/502	2.13	22/677 (3.2%)
All	All	1.00	0/2815	1.93	83/3787 (2.2%)

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	H	0	2
3	I	0	4
All	All	0	6

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	93	ARG	NE-CZ-NH2	-11.83	114.38	120.30
1	H	99	TYR	CB-CG-CD2	-10.78	114.53	121.00
1	H	127	TRP	CD1-CG-CD2	9.06	113.55	106.30
1	H	237	TRP	CD1-CG-CD2	8.80	113.34	106.30
1	H	215	TRP	CD1-CG-CD2	8.69	113.25	106.30
1	H	115	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	H	29	TRP	CD1-CG-CD2	8.30	112.94	106.30
2	L	439	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	I	503	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	L	439	ARG	NE-CZ-NH1	8.17	124.38	120.30
3	I	511	TRP	CG-CD2-CE3	8.02	141.12	133.90
1	H	237	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	H	127	TRP	CE2-CD2-CG	-7.88	101.00	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	215	TRP	CE2-CD2-CG	-7.83	101.04	107.30
1	H	29	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	H	168	CYS	CA-CB-SG	7.71	127.88	114.00
3	I	537	TRP	CE2-CD2-CG	-7.60	101.22	107.30
3	I	501	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	H	93	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	H	107	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	H	159	GLU	N-CA-CB	-7.31	97.44	110.60
1	H	113	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	H	29	TRP	CG-CD2-CE3	7.22	140.40	133.90
1	H	165	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	L	438	GLY	CA-C-N	-7.20	101.36	117.20
3	I	537	TRP	CD1-CG-CD2	7.07	111.96	106.30
1	H	240	LYS	CA-CB-CG	7.02	128.85	113.40
1	H	185	TYR	N-CA-C	6.53	128.63	111.00
3	I	543	HIS	CA-CB-CG	6.51	124.67	113.60
3	I	511	TRP	CA-CB-CG	6.36	125.78	113.70
3	I	511	TRP	CE2-CD2-CG	-6.35	102.22	107.30
1	H	209	VAL	CA-CB-CG2	-6.32	101.42	110.90
3	I	511	TRP	CA-C-N	6.32	131.10	117.20
2	L	427	THR	CA-C-N	-6.24	103.47	117.20
1	H	228	TYR	CB-CG-CD1	-6.13	117.32	121.00
3	I	503	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	H	222	ARG	CG-CD-NE	-6.03	99.13	111.80
1	H	149	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	H	149	ARG	CA-C-N	-5.97	104.06	117.20
3	I	535	SER	N-CA-C	-5.96	94.90	111.00
1	H	127	TRP	CG-CD1-NE1	-5.92	104.18	110.10
1	H	237	TRP	CG-CD1-NE1	-5.91	104.19	110.10
1	H	237	TRP	CB-CG-CD1	-5.87	119.37	127.00
1	H	237	TRP	CG-CD2-CE3	5.79	139.11	133.90
1	H	96	LYS	N-CA-C	5.77	126.57	111.00
3	I	537	TRP	CG-CD2-CE3	5.74	139.07	133.90
1	H	235	LEU	CB-CG-CD1	-5.70	101.30	111.00
1	H	99	TYR	CB-CG-CD1	5.66	124.39	121.00
3	I	511	TRP	CB-CG-CD1	-5.65	119.66	127.00
1	H	222	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	H	165	ARG	NE-CZ-NH1	5.63	123.12	120.30
3	I	547	ASP	CB-CG-OD2	5.63	123.37	118.30
3	I	527	ARG	NE-CZ-NH2	-5.55	117.53	120.30
3	I	554	ASP	CB-CG-OD1	5.54	123.29	118.30
1	H	113	ARG	N-CA-C	-5.52	96.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	29	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	H	96	LYS	CA-C-N	5.49	129.27	117.20
3	I	547	ASP	CA-CB-CG	5.46	125.42	113.40
1	H	231	VAL	CA-CB-CG2	-5.42	102.77	110.90
3	I	511	TRP	NE1-CE2-CZ2	-5.41	124.45	130.40
1	H	29	TRP	CB-CG-CD1	-5.38	120.01	127.00
2	L	438	GLY	O-C-N	5.37	131.29	122.70
1	H	205	ASP	CA-CB-CG	-5.36	101.61	113.40
1	H	180	MET	CA-CB-CG	5.35	122.39	113.30
1	H	115	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	H	92	SER	CA-C-N	-5.32	105.50	117.20
3	I	553	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	H	215	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	H	122	CYS	CA-CB-SG	5.28	123.50	114.00
1	H	124(A)	GLU	OE1-CD-OE2	-5.24	117.02	123.30
2	L	431	PRO	N-CD-CG	-5.22	95.37	103.20
1	H	39	GLU	CA-CB-CG	-5.21	101.93	113.40
3	I	549	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	H	33	LEU	N-CA-C	-5.19	97.00	111.00
1	H	231	VAL	CA-CB-CG1	5.15	118.63	110.90
1	H	215	TRP	CB-CG-CD1	-5.13	120.33	127.00
2	L	436	THR	CA-CB-CG2	-5.12	105.22	112.40
2	L	438	GLY	N-CA-C	5.10	125.86	113.10
1	H	149	ARG	N-CA-C	5.10	124.76	111.00
1	H	205	ASP	N-CA-C	5.10	124.76	111.00
3	I	537	TRP	CA-C-N	-5.07	106.04	117.20
2	L	437	GLN	O-C-N	5.06	131.80	123.20
3	I	525	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	228	TYR	Sidechain
1	H	247	GLY	Peptide
3	I	506	ILE	Peptide
3	I	507	LYS	Peptide
3	I	529	GLY	Mainchain
3	I	552	TYR	Sidechain

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	H	1880	0	1828	74	4
2	L	388	0	346	12	2
3	I	488	0	418	19	6
All	All	2756	0	2592	100	6

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 19.

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:H:94:PHE:HE2	1:H:96:LYS:HZ2	1.04	1.00
1:H:35:ASN:HD21	1:H:61(A):ALA:HA	1.47	0.79
2:L:415:TYR:HB3	2:L:424:CYS:HB3	1.65	0.79
1:H:185(B):THR:HA	1:H:223:LYS:HD2	1.65	0.78
2:L:400:CYS:SG	2:L:407:VAL:HB	2.24	0.77
1:H:185:TYR:HB3	1:H:186:GLN:HB3	1.68	0.75
1:H:41:PHE:CZ	1:H:61(A):ALA:HB2	2.22	0.74
1:H:239:ASP:HA	1:H:242:MET:HB2	1.71	0.72
3:I:509:ARG:NH1	3:I:511:TRP:HA	2.04	0.71
1:H:30:GLN:HG3	1:H:155:LEU:HD11	1.72	0.71
1:H:237:TRP:HA	1:H:240:LYS:HE2	1.73	0.69
1:H:67:ARG:HA	1:H:82:ALA:HA	1.75	0.69
3:I:540:PRO:HA	3:I:543:HIS:ND1	2.09	0.68
1:H:86:GLU:HB2	1:H:109:LYS:HG2	1.76	0.67
1:H:212:ILE:HB	1:H:229:THR:HB	1.75	0.67
1:H:26:GLU:O	1:H:28:PRO:HD3	1.94	0.66
2:L:437:GLN:NE2	2:L:438:GLY:H	1.93	0.65
1:H:73:THR:O	1:H:76:GLU:HG2	1.96	0.65
1:H:147:LYS:HG3	3:I:558:ALA:HB2	1.79	0.65
3:I:524:ALA:HB3	3:I:526:PHE:CE1	2.32	0.65
3:I:556:PHE:HA	3:I:560:ILE:HD13	1.79	0.64
1:H:27:CYS:HB2	1:H:155:LEU:HD21	1.83	0.60
1:H:202:ARG:NH2	1:H:204:LYS:HA	2.17	0.60
3:I:556:PHE:HA	3:I:560:ILE:CD1	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:506:ILE:HB	3:I:508:PRO:HG3	1.85	0.58
1:H:62:LYS:HA	1:H:62:LYS:HE3	1.85	0.58
1:H:202:ARG:HB3	1:H:207:TYR:CE1	2.38	0.58
3:I:528:ASN:HB3	3:I:534:ASP:HB3	1.87	0.57
1:H:202:ARG:HH21	1:H:204:LYS:HA	1.70	0.56
1:H:74:GLU:H	1:H:153:SER:HG	1.53	0.55
2:L:437:GLN:HE21	2:L:438:GLY:H	1.53	0.55
1:H:206:THR:HA	2:L:433:GLY:O	2.05	0.55
1:H:73:THR:HB	1:H:153:SER:OG	2.07	0.55
1:H:241:ILE:HA	1:H:244:ALA:O	2.07	0.55
1:H:185(B):THR:HA	1:H:223:LYS:CD	2.34	0.54
1:H:22:CYS:SG	1:H:157:MET:HB3	2.48	0.53
1:H:51:TYR:HB3	1:H:105:VAL:HG12	1.90	0.53
1:H:197:GLY:O	1:H:213:VAL:HG23	2.07	0.53
3:I:511:TRP:O	3:I:512:ILE:HB	2.09	0.53
1:H:120:PRO:O	2:L:432:CYS:HA	2.08	0.52
3:I:521:GLY:HA2	3:I:538:ILE:O	2.08	0.52
1:H:95:VAL:HB	1:H:98:THR:HB	1.92	0.52
1:H:35:ASN:HA	1:H:63:ARG:O	2.10	0.51
3:I:511:TRP:CE3	3:I:542:ASP:HB3	2.45	0.51
1:H:84:GLU:CD	1:H:109:LYS:HZ3	2.13	0.51
1:H:36:GLU:HG3	1:H:63:ARG:H	1.75	0.51
1:H:101:PHE:HA	1:H:234:PHE:CZ	2.47	0.50
2:L:395:GLY:O	2:L:422:LYS:HB3	2.11	0.50
1:H:202:ARG:HB3	1:H:207:TYR:CZ	2.47	0.50
1:H:147:LYS:HZ2	3:I:554:ASP:CG	2.15	0.50
1:H:18:GLY:O	1:H:156:LYS:NZ	2.45	0.50
1:H:85:VAL:HG22	1:H:108:LEU:HD23	1.94	0.50
1:H:143:ARG:HD3	1:H:148:GLY:O	2.12	0.49
1:H:58:CYS:HA	1:H:61:GLN:HE21	1.78	0.49
1:H:46:ILE:HD11	1:H:68:VAL:HG13	1.93	0.49
1:H:51:TYR:HB3	1:H:105:VAL:CG1	2.43	0.49
1:H:74:GLU:N	1:H:153:SER:OG	2.42	0.49
1:H:47:LEU:HD11	1:H:53:LEU:HG	1.93	0.48
1:H:185(A):ASP:OD1	1:H:223(A):GLY:HA2	2.12	0.48
1:H:174:PHE:HE1	1:H:217:GLU:HG2	1.78	0.48
1:H:146:GLU:HB2	1:H:220:CYS:HB2	1.95	0.48
2:L:417:LEU:HA	2:L:423:SER:O	2.14	0.48
1:H:28:PRO:HD2	1:H:29:TRP:CD2	2.49	0.47
3:I:520:GLY:O	3:I:540:PRO:HG3	2.14	0.47
1:H:92:SER:HB2	1:H:251:SER:OXT	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:PHE:HA	1:H:100:ASP:O	2.14	0.47
2:L:437:GLN:NE2	2:L:438:GLY:N	2.61	0.47
1:H:72:ASN:HB2	1:H:75:GLN:NE2	2.30	0.47
3:I:511:TRP:HB2	3:I:513:ASP:OD1	2.15	0.47
3:I:549:TYR:CE2	3:I:559:CYS:SG	3.08	0.47
1:H:223:LYS:HA	1:H:223:LYS:HD3	1.86	0.45
1:H:93:ARG:NH2	1:H:250:GLY:O	2.50	0.45
1:H:185(A):ASP:HB2	1:H:225:PHE:CE1	2.52	0.44
1:H:131(A):LEU:HD21	1:H:203:PHE:HB2	1.99	0.44
2:L:437:GLN:HE21	2:L:437:GLN:HB2	1.32	0.44
1:H:52:VAL:HG21	1:H:66:VAL:HG11	2.00	0.44
1:H:97:GLU:O	3:I:503:ARG:NH2	2.51	0.43
1:H:186:GLN:HA	1:H:187:PRO:HD3	1.79	0.43
1:H:57:HIS:HD2	1:H:102:ASP:OD2	2.00	0.43
1:H:114:PHE:HA	1:H:118:VAL:HB	1.99	0.43
1:H:94:PHE:CD1	1:H:102:ASP:HA	2.54	0.43
1:H:234:PHE:O	1:H:238:ILE:HG13	2.17	0.43
3:I:520:GLY:O	3:I:543:HIS:CE1	2.72	0.43
1:H:138:VAL:HA	1:H:198:PRO:O	2.19	0.43
2:L:414:GLY:O	2:L:427:THR:HB	2.19	0.42
1:H:89:VAL:HG22	1:H:246:ALA:O	2.19	0.42
1:H:43:GLY:O	1:H:196:GLY:HA3	2.19	0.42
3:I:541:GLU:H	3:I:541:GLU:CD	2.23	0.42
1:H:57:HIS:O	1:H:61:GLN:NE2	2.53	0.42
1:H:202:ARG:HA	1:H:207:TYR:HA	2.00	0.42
1:H:171:SER:O	1:H:224:LYS:HE2	2.19	0.42
1:H:141:PHE:HB3	1:H:152:SER:O	2.20	0.42
1:H:200:VAL:HA	1:H:208:PHE:O	2.20	0.42
2:L:401:ARG:O	2:L:407:VAL:HA	2.19	0.41
1:H:222:ARG:HB3	1:H:224:LYS:HB2	2.01	0.41
1:H:94:PHE:HE2	1:H:96:LYS:NZ	1.92	0.41
1:H:84:GLU:OE1	1:H:109:LYS:NZ	2.53	0.41
1:H:101:PHE:HA	1:H:234:PHE:HZ	1.85	0.41
1:H:131(B):MET:HG2	1:H:162:TYR:CE2	2.55	0.41
3:I:509:ARG:CZ	3:I:511:TRP:HA	2.51	0.41

All (6) 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)
1:H:233:ASN:O	3:I:518:ASN:ND2[3_655]	1.32	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ASN:O	3:I:518:ASN:CG[3_655]	1.85	0.35
2:L:401:ARG:NH2	3:I:535:SER:OG[3_655]	1.97	0.23
1:H:233:ASN:C	3:I:518:ASN:ND2[3_655]	2.06	0.14
1:H:233:ASN:O	3:I:518:ASN:OD1[3_655]	2.17	0.03
2:L:404:ARG:NH1	3:I:556:PHE:CD2[3_655]	2.18	0.02

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	H	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	2 14
2	L	49/51 (96%)	32 (65%)	9 (18%)	8 (16%)	0 1
3	I	58/60 (97%)	37 (64%)	13 (22%)	8 (14%)	0 1
All	All	346/352 (98%)	259 (75%)	58 (17%)	29 (8%)	1 5

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	60	HIS
1	H	73	THR
1	H	79	ASN
1	H	93	ARG
2	L	421	SER
2	L	428	GLU
3	I	512	ILE
3	I	529	GLY
3	I	535	SER
3	I	555	CYS
1	H	19	GLY
1	H	26	GLU
1	H	81	MET
2	L	392	ASP

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Mol	Chain	Res	Type
2	L	405	SER
3	I	510	ASP
1	H	185(A)	ASP
1	H	245	ARG
1	H	248	ALA
2	L	404	ARG
3	I	509	ARG
1	H	94	PHE
2	L	390	SER
2	L	398	GLN
3	I	547	ASP
1	H	80	GLU
3	I	530	LYS
1	H	187	PRO
2	L	393	ASN

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	H	200/200 (100%)	170 (85%)	30 (15%)	3 17
2	L	44/44 (100%)	37 (84%)	7 (16%)	3 15
3	I	51/51 (100%)	38 (74%)	13 (26%)	1 3
All	All	295/295 (100%)	245 (83%)	50 (17%)	2 13

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	21	ASP
1	H	28	PRO
1	H	29	TRP
1	H	30	GLN
1	H	32	LEU
1	H	37	GLU
1	H	49	GLU

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Mol	Chain	Res	Type
1	H	54	THR
1	H	61	GLN
1	H	62	LYS
1	H	64	PHE
1	H	75	GLN
1	H	84	GLU
1	H	86	GLU
1	H	91	HIS
1	H	106	LEU
1	H	110	THR
1	H	113	ARG
1	H	124(A)	GLU
1	H	125	LYS
1	H	144	THR
1	H	147	LYS
1	H	156	LYS
1	H	164	ASP
1	H	169	LYS
1	H	175	THR
1	H	185(B)	THR
1	H	223	LYS
1	H	233	ASN
1	H	245	ARG
2	L	396	CYS
2	L	398	GLN
2	L	419	ASP
2	L	429	ARG
2	L	435	PHE
2	L	436	THR
2	L	437	GLN
3	I	503	ARG
3	I	507	LYS
3	I	511	TRP
3	I	513	ASP
3	I	518	ASN
3	I	519	GLU
3	I	522	GLU
3	I	538	ILE
3	I	542	ASP
3	I	550	SER
3	I	551	SER
3	I	553	ARG

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Mol	Chain	Res	Type
3	I	557	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	57	HIS
1	H	83	HIS
2	L	437	GLN

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.