

Full wwPDB X-ray Structure Validation Report (i)

Aug 2, 2023 – 02:17 AM EDT

PDB ID	:	1C5M
Title	:	STRUCTURAL BASIS FOR SELECTIVITY OF A SMALL MOLECULE,
		S1-BINDING, SUB-MICROMOLAR INHIBITOR OF UROKINASE TYPE
		PLASMINOGEN ACTIVATOR
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Deposited on	:	1999-12-22
Resolution	:	1.95 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 1.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678(1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain			
1	D	255	60%		27%	5% • 5%
2	F	96	32% 14	4% 7% •	46%	



1C5M

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5896 atoms, of which 3142 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 PROTEIN (COAGULATION FACTOR X).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	D	241	Total 3786	C 1201	Н 1879	N 335	O 357	S 14	68	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	257	VAL	-	insertion	UNP P00742

• Molecule 2 is a protein called PROTEIN (COAGULATION FACTOR X).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	F	52	Total 748	C 235	Н 355	N 70	0 81	${f S}{7}$	26	1	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	354	Total 1062	Н 708	O 354	0	9
3	F	100	Total 300	Н 200	O 100	0	1



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Chain D:	60%	27%	5% • 5%
116 417 618 619 619 825 838 838 838 838 838 838 838 838 838 83	F64 K65 R67 R71 R71 R71 R71 R71 E76 E76 E76 E76 E76 E76 E76 E76 R90 K90 K90 K91 K93 K93	E97 198 799 F101 D102 R107	R115 M116 C122 C122 R125 U127 W127 L131A M1318
1132 4133 K134 T135 S139 S139 C142 R144 T144 F144 F144 F144 F144 F144 F146 F146 F	L158 1159 1161 1162 1162 1176 1176 1176 1176 1177 1176 1178 1177 11858 11858	K186 Q187 S195 G196 G197 P198 H199	R202 F203 F203 K204 D205 V209 V209 W215
R222 1227 1227 1227 1236 1236 1238 1238 1238 1238 1238 1238 1238 1238	A250 K251 SER HIS FIA ALA ALA ALA CLU CLU LYS LYS		
• Molecule 2: PROTEIN	(COAGULATION FACTOR	(X)	
Chain F: 32%	14% 7% .	46%	
TTR LVS LVS ASP ASP CTS CTS CTS CTS CTS CTS CTS CTS CTS CTS	ASP GLY CLU CLU CLY CLY CLY CLY CLY CLY CLY CLY CLY CLY	PHE THR ARG LVS CI CS CI SS CI	D7 E14 N17 S18 S18 S22 R25 C26
T27 T28 N32 N32 C35 C35 T39 T39 T39 T39 T39 T39 T39 T39 T39 T39			

• Molecule 1: PROTEIN (COAGULATION FACTOR X)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	81.82Å 81.82Å 108.79Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	7.50 - 1.95	Depositor
Resolution (A)	33.69 - 1.64	EDS
% Data completeness	60.4(7.50-1.95)	Depositor
(in resolution range)	41.6(33.69-1.64)	EDS
R _{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.53 (at 1.64 \text{\AA})$	Xtriage
Refinement program	X-PLOR 3.1	Depositor
D D.	0.218 , 0.307	Depositor
Π, Π_{free}	0.269 , (Not available)	DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor $(Å^2)$	13.2	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.28 , 64.5	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5896	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 4.37% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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		Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	D	1.42	7/1950~(0.4%)	1.68	38/2625~(1.4%)	
2	F	1.36	0/404	1.52	1/545~(0.2%)	
All	All	1.41	7/2354~(0.3%)	1.65	39/3170~(1.2%)	

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	D	0	14
2	F	0	2
All	All	0	16

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	D	196	GLY	C-N	-6.38	1.21	1.33
1	D	76	GLU	CD-OE2	6.20	1.32	1.25
1	D	76	GLU	CG-CD	5.72	1.60	1.51
1	D	76	GLU	CD-OE1	-5.43	1.19	1.25
1	D	237	TRP	CG-CD2	-5.39	1.34	1.43
1	D	127	TRP	CG-CD2	-5.09	1.34	1.43
1	D	29	TRP	CG-CD2	-5.03	1.35	1.43

All (7) bond length outliers are listed below:

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	D	76	GLU	OE1-CD-OE2	17.68	144.52	123.30
1	D	215	TRP	CD1-NE1-CE2	10.29	118.27	109.00
1	D	127	TRP	CD1-NE1-CE2	9.72	117.75	109.00
1	D	237	TRP	CD1-NE1-CE2	9.27	117.34	109.00
1	D	115	ARG	NE-CZ-NH2	-8.99	115.81	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	215	TRP	NE1-CE2-CZ2	8.55	139.80	130.40
1	D	237	TRP	CG-CD1-NE1	-8.14	101.96	110.10
1	D	29	TRP	CD1-NE1-CE2	8.06	116.25	109.00
1	D	237	TRP	NE1-CE2-CZ2	7.97	139.17	130.40
1	D	29	TRP	NE1-CE2-CZ2	7.58	138.74	130.40
1	D	127	TRP	CG-CD1-NE1	-7.54	102.56	110.10
1	D	215	TRP	CG-CD1-NE1	-6.98	103.12	110.10
1	D	76	GLU	CG-CD-OE1	-6.95	104.40	118.30
1	D	99	TYR	CB-CG-CD2	-6.91	116.85	121.00
1	D	215	TRP	NE1-CE2-CD2	-6.85	100.45	107.30
1	D	127	TRP	NE1-CE2-CZ2	6.67	137.74	130.40
1	D	199	HIS	N-CA-C	-6.56	93.28	111.00
1	D	107	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	D	29	TRP	CG-CD1-NE1	-6.20	103.90	110.10
1	D	248	PRO	N-CA-C	6.10	127.95	112.10
1	D	127	TRP	NE1-CE2-CD2	-5.95	101.36	107.30
1	D	19	GLY	N-CA-C	-5.89	98.39	113.10
1	D	237	TRP	NE1-CE2-CD2	-5.79	101.52	107.30
1	D	29	TRP	NE1-CE2-CD2	-5.58	101.72	107.30
1	D	185	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	D	176	ILE	N-CA-C	-5.49	96.17	111.00
1	D	102	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	D	135	THR	N-CA-CB	-5.41	100.03	110.30
2	F	14	GLU	N-CA-C	-5.34	96.59	111.00
1	D	39	GLU	N-CA-C	-5.31	96.66	111.00
1	D	107	ARG	N-CA-C	-5.28	96.73	111.00
1	D	203	PHE	N-CA-C	-5.24	96.85	111.00
1	D	71	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	D	222	ARG	N-CA-C	-5.22	96.90	111.00
1	D	115	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	212	ILE	N-CA-C	-5.12	97.18	111.00
1	D	63	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	199	HIS	CA-CB-CG	-5.03	105.05	113.60
1	D	168	CYS	CA-CB-SG	5.02	123.04	114.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	115	ARG	Sidechain
1	D	125	ARG	Sidechain
1	D	143	ARG	Sidechain



Mol	Chain	Res	Type	Group
1	D	150	ARG	Sidechain
1	D	154	ARG	Sidechain
1	D	165	ARG	Sidechain
1	D	202	ARG	Sidechain
1	D	222	ARG	Sidechain
1	D	240	ARG	Sidechain
1	D	245	ARG	Sidechain
1	D	247	LEU	Peptide
1	D	63	ARG	Sidechain
1	D	67	ARG	Sidechain
1	D	93	ARG	Sidechain
2	F	25	ARG	Sidechain
2	F	51	ARG	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	D	1907	1879	1874	46	4
2	F	393	355	355	20	12
3	D	354	708	0	11	45
3	F	100	200	0	14	21
All	All	2754	3142	2229	64	49

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 14.

All (64) 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)
2:F:7:ASP:HA	3:F:71:HOH:O	1.13	1.26
1:D:187:GLN:HG2	3:D:427:HOH:O	1.07	1.21
2:F:0:LEU:HG	3:F:77:HOH:O	0.97	1.14
1:D:93:ARG:HG2	3:D:602:HOH:O	0.91	1.07
1:D:92:ASN:ND2	3:D:602:HOH:O	1.97	0.97
1:D:90:LYS:NZ	3:D:300:HOH:O	1.57	0.96



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:F:1:CYS:O	3:F:76:HOH:O	1.84	0.93
2:F:7:ASP:CB	3:F:71:HOH:O	2.13	0.89
1:D:92:ASN:O	3:D:601:HOH:O	1.98	0.81
2:F:7:ASP:CG	3:F:71:HOH:O	2.18	0.81
1:D:93:ARG:CG	3:D:602:HOH:O	1.65	0.80
2:F:14:GLU:OE1	3:F:92:HOH:O	2.11	0.69
2:F:3:LEU:HD23	3:F:107:HOH:O	1.93	0.69
1:D:91:HIS:CE1	3:D:602:HOH:O	2.47	0.67
1:D:131(B):MET:HE2	1:D:162:TYR:CE1	2.35	0.62
2:F:7:ASP:CA	3:F:71:HOH:O	1.86	0.61
1:D:215:TRP:CE2	1:D:227:ILE:HG12	2.37	0.59
1:D:247:LEU:HG	1:D:248:PRO:HD3	1.84	0.59
2:F:0:LEU:N	3:F:77:HOH:O	2.28	0.57
1:D:92:ASN:HD21	1:D:250:ALA:HB2	1.71	0.56
1:D:92:ASN:N	1:D:92:ASN:HD22	2.03	0.56
1:D:16:ILE:N	1:D:142:GLY:O	2.39	0.56
1:D:93:ARG:HD2	3:D:601:HOH:O	2.06	0.54
1:D:93:ARG:CD	3:D:601:HOH:O	2.55	0.53
1:D:125:ARG:H	1:D:235:LEU:HD23	1.74	0.53
2:F:0:LEU:CG	3:F:77:HOH:O	1.84	0.52
1:D:93:ARG:N	3:D:602:HOH:O	2.44	0.51
1:D:131(B):MET:HE2	1:D:162:TYR:CZ	2.46	0.50
1:D:131(B):MET:CE	1:D:162:TYR:CE1	2.95	0.50
2:F:14:GLU:CG	3:F:74:HOH:O	0.81	0.49
1:D:247:LEU:HG	1:D:248:PRO:CD	2.44	0.48
1:D:240:ARG:NH2	1:D:251:LYS:HB3	2.28	0.48
2:F:38:PRO:HB3	2:F:43:PRO:HG3	1.97	0.47
2:F:14:GLU:HG3	3:F:74:HOH:O	0.61	0.47
1:D:45:THR:OG1	1:D:198:PRO:HB3	2.15	0.47
1:D:247:LEU:HB3	1:D:248:PRO:HD2	1.97	0.46
1:D:215:TRP:NE1	1:D:227:ILE:HD11	2.31	0.45
1:D:45:THR:HG21	1:D:209:VAL:HG11	1.98	0.44
1:D:25:GLY:HA2	2:F:48:THR:OG1	2.18	0.43
1:D:51:TYR:CD2	1:D:51:TYR:N	2.86	0.43
1:D:234:PHE:O	1:D:238:ILE:HG13	2.18	0.43
1:D:240:ARG:HH22	1:D:251:LYS:HB3	1.82	0.43
2:F:32:ASN:ND2	2:F:34:LYS:HB2	2.33	0.43
1:D:72:ASN:HD22	1:D:75:GLN:CB	2.31	0.43
1:D:158:LEU:HD13	1:D:160:VAL:HG13	2.01	0.43
1:D:93:ARG:CB	3:D:602:HOH:O	2.32	0.43
1:D:125:ARG:N	1:D:235:LEU:HD23	2.33	0.43



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:D:203:PHE:O	1:D:204:LYS:C	2.57	0.43
2:F:3:LEU:CD2	3:F:107:HOH:O	2.62	0.43
1:D:16:ILE:N	1:D:143:ARG:O	2.51	0.43
2:F:1:CYS:O	2:F:2:SER:C	2.58	0.43
1:D:247:LEU:CB	1:D:248:PRO:HD2	2.49	0.42
1:D:72:ASN:HA	1:D:153:THR:O	2.20	0.42
1:D:90:LYS:O	1:D:248:PRO:HA	2.20	0.41
1:D:131(A):LEU:O	1:D:133:GLN:HB2	2.20	0.41
1:D:248:PRO:O	1:D:249:LYS:HG2	2.20	0.41
1:D:122:CYS:SG	2:F:44:CYS:O	2.78	0.41
1:D:150:ARG:NH1	1:D:150:ARG:CG	2.84	0.41
1:D:135:THR:HA	1:D:161:PRO:HA	2.02	0.41
1:D:165:ARG:HH22	1:D:230:LYS:NZ	2.19	0.41
2:F:3:LEU:CG	3:F:107:HOH:O	2.68	0.41
2:F:27:TYR:HB3	2:F:36:CYS:HB3	2.04	0.40
1:D:165:ARG:HH21	1:D:178:GLN:HA	1.87	0.40
1:D:91:HIS:CE1	1:D:101:PHE:CD2	3.10	0.40

All (49) 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	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:119[C]:HOH:O	3:F:119[C]:HOH:O[5_675]	0.42	1.78
3:D:302:HOH:H1	3:D:500:HOH:H2[4_566]	0.44	1.16
3:D:482:HOH:O	3:F:67:HOH:O[5_675]	1.04	1.16
3:D:482:HOH:H1	3:F:67:HOH:O[5_675]	0.51	1.09
3:D:482:HOH:O	3:F:67:HOH:H2[5_675]	0.55	1.05
3:D:375:HOH:O	3:F:140:HOH:O[2_665]	1.19	1.01
2:F:0:LEU:HD13	3:D:305:HOH:H2[4_456]	0.69	0.91
3:F:119[C]:HOH:H1	3:F:119[C]:HOH:H1[5_675]	0.71	0.89
3:D:439:HOH:H1	3:F:151:HOH:H1[4_556]	0.80	0.80
3:D:302:HOH:H2	3:D:500:HOH:H1[4_566]	0.81	0.79
3:D:584:HOH:H2	3:D:604:HOH:H2[4_556]	0.82	0.78
3:D:482:HOH:H2	3:F:67:HOH:H2[5_675]	0.88	0.72
3:F:119[C]:HOH:O	3:F:119[C]:HOH:H1[5_675]	0.88	0.72
3:D:375:HOH:H1	3:F:140:HOH:O[2_665]	0.91	0.69
2:F:18:SER:OG	3:D:514:HOH:O[5_675]	1.53	0.67
3:D:302:HOH:O	3:D:500:HOH:H2[4_566]	0.97	0.63
3:D:302:HOH:O	3:D:500:HOH:O[4_566]	1.57	0.63
3:D:439:HOH:O	3:F:151:HOH:H1[4_556]	0.97	0.63



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:134:LYS:HB2	3:D:360:HOH:H2[4_456]	1.05	0.55
3:D:482:HOH:H1	3:F:67:HOH:H2[5_675]	1.07	0.53
3:D:439:HOH:H1	3:F:151:HOH:O[4_556]	1.09	0.51
2:F:0:LEU:HD13	3:D:305:HOH:O[4_456]	1.11	0.49
3:D:375:HOH:H2	3:F:140:HOH:O[2_665]	1.11	0.49
3:D:375:HOH:H2	3:F:140:HOH:H1[2_665]	1.12	0.48
3:D:584:HOH:H2	3:D:604:HOH:O[4_556]	1.12	0.48
1:D:134:LYS:HB2	3:D:360:HOH:O[4_456]	1.13	0.47
2:F:0:LEU:HD12	3:D:305:HOH:H1[4_456]	1.14	0.46
3:D:340:HOH:H2	3:D:516:HOH:H1[4_556]	1.15	0.45
2:F:18:SER:OG	3:D:514:HOH:H2[5_675]	1.16	0.44
3:D:388:HOH:O	3:F:114:HOH:H2[5_675]	1.18	0.42
3:D:439:HOH:O	3:F:151:HOH:O[4_556]	1.79	0.41
3:D:302:HOH:H2	3:D:500:HOH:O[4_566]	1.20	0.40
3:D:302:HOH:H2	3:D:500:HOH:H2[4_566]	1.23	0.37
2:F:0:LEU:CD1	3:D:305:HOH:O[4_456]	1.83	0.37
3:D:388:HOH:O	3:F:114:HOH:O[5_675]	1.87	0.33
1:D:65:LYS:HZ2	3:D:375:HOH:O[4_566]	1.29	0.31
3:D:482:HOH:H2	3:F:67:HOH:O[5_675]	1.30	0.30
2:F:0:LEU:HD12	3:D:286:HOH:O[4_456]	1.38	0.22
3:F:119[C]:HOH:O	3:F:119[C]:HOH:H2[5_675]	1.38	0.22
3:D:302:HOH:H1	3:D:500:HOH:O[4_566]	1.40	0.20
2:F:0:LEU:CD1	3:D:305:HOH:H2[4_456]	1.43	0.17
3:D:584:HOH:O	3:D:604:HOH:O[4_556]	2.03	0.17
1:D:65:LYS:NZ	3:D:375:HOH:O[4_566]	2.06	0.14
2:F:39:THR:O	3:D:387:HOH:H2[5_675]	1.48	0.12
3:D:302:HOH:O	3:D:500:HOH:H1[4_566]	1.50	0.10
2:F:0:LEU:H	3:D:504:HOH:O[4_456]	1.51	0.09
2:F:18:SER:OG	3:D:514:HOH:H1[5_675]	1.51	0.09
3:D:375:HOH:O	3:F:140:HOH:H1[2_665]	1.55	0.05
2:F:0:LEU:N	3:D:504:HOH:O[4_456]	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	D	240/255~(94%)	202 (84%)	25 (10%)	13~(5%)	2 0
2	F	51/96~(53%)	38 (74%)	8 (16%)	5 (10%)	0 0
All	All	291/351 (83%)	240 (82%)	33 (11%)	18 (6%)	1 0

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	36	GLU
1	D	125	ARG
2	F	7	ASP
1	D	18	GLY
1	D	73	THR
1	D	80	GLU
1	D	143	ARG
1	D	151	GLN
1	D	204	LYS
1	D	205	ASP
1	D	249	LYS
2	F	3	LEU
1	D	248	PRO
2	F	2	SER
1	D	182	CYS
2	F	1	CYS
1	D	146	GLU
2	F	43	PRO

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	D	205/217~(94%)	182~(89%)	23~(11%)	6 1
2	F	45/82~(55%)	39~(87%)	6 (13%)	4 0
All	All	250/299~(84%)	221 (88%)	29 (12%)	6 1

All (29) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	D	37	GLU
1	D	63	ARG
1	D	73	THR
1	D	74	GLU
1	D	88	VAL
1	D	92	ASN
1	D	97	GLU
1	D	98	THR
1	D	116	MET
1	D	125	ARG
1	D	132	THR
1	D	133	GLN
1	D	139	SER
1	D	144	THR
1	D	150	ARG
1	D	165	ARG
1	D	173	SER
1	D	185(B)	THR
1	D	195[A]	SER
1	D	195[B]	SER
1	D	235	LEU
1	D	245	ARG
1	D	249	LYS
2	F	2	SER
2	F	17	ASN
2	F	22	SER
2	F	28	THR
2	F	39	THR
2	F	51	ARG

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

Mol	Chain	Res	Type
1	D	30	GLN
1	D	38	ASN
1	D	92	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

