



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:12 PM UTC

PDB ID : 1C5M / pdb_00001c5m
Title : STRUCTURAL BASIS FOR SELECTIVITY OF A SMALL MOLECULE,
S1-BINDING, SUB-MICROMOLAR INHIBITOR OF UROKINASE TYPE
PLASMINOGEN ACTIVATOR
Authors : Katz, B.A.; Mackman, R.; Luong, C.; Radika, K.; Martelli, A.; Sprengeler,
P.A.; Wang, J.; Chan, H.; Wong, L.
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

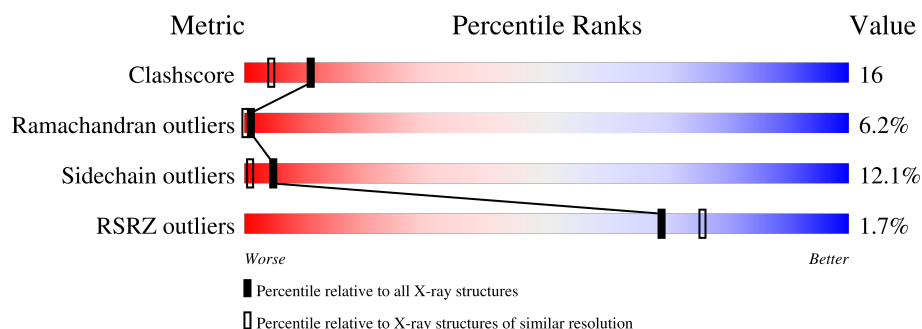
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 $\leq 5\%$. 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	D	255	2% 44% 38% 9% • 5%
2	F	96	% 23% 22% 7% • 46%

2 Entry composition

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	C	H	N	O	S	68	1	0
			3786	1201	1879	335	357	14			

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	C	H	N	O	S	26	1	0
			748	235	355	70	81	7			

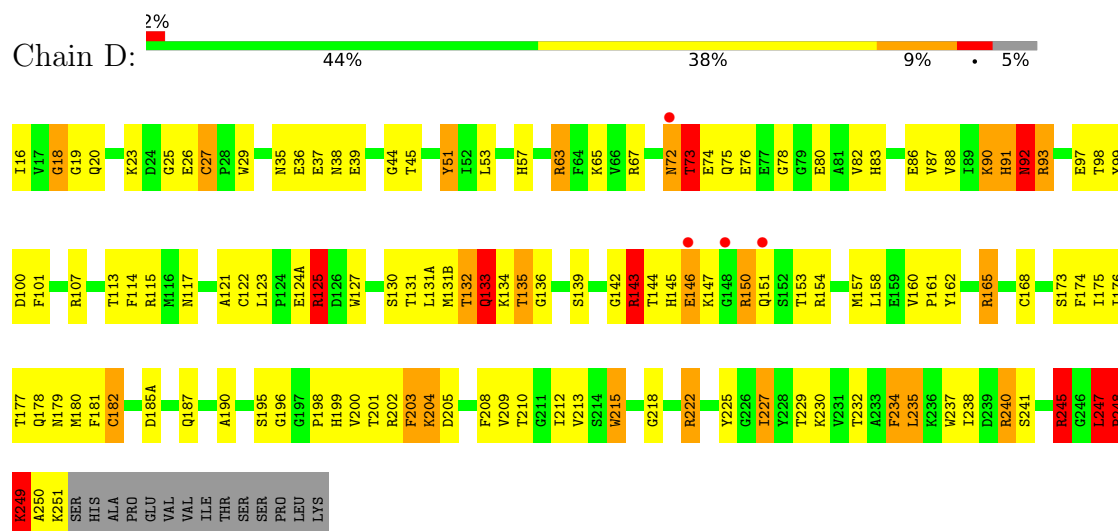
- Molecule 3 is water.

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

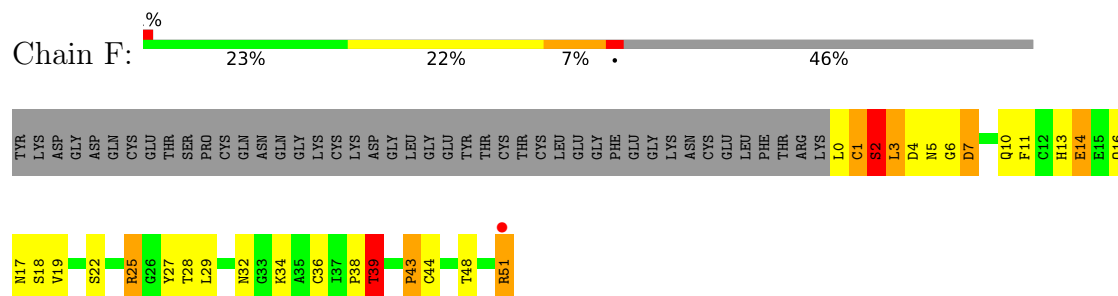
3 Residue-property plots [i](#)

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 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: PROTEIN (COAGULATION FACTOR X)



- Molecule 2: PROTEIN (COAGULATION FACTOR X)



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.82Å 81.82Å 108.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	7.50 – 1.95 7.50 – 1.95	Depositor EDS
% Data completeness (in resolution range)	60.4 (7.50-1.95) 60.4 (7.50-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.64Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.218 , 0.307 0.267 , (Not available)	Depositor 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)	0.29 , 70.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

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.

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	D	1.92	21/1950 (1.1%)	2.04	73/2625 (2.8%)
2	F	1.87	4/404 (1.0%)	2.04	14/545 (2.6%)
All	All	1.91	25/2354 (1.1%)	2.04	87/3170 (2.7%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	HIS	CG-ND1	-8.44	1.28	1.38
1	D	145	HIS	CG-ND1	-8.27	1.29	1.38
1	D	57	HIS	CG-ND1	-8.18	1.29	1.38
1	D	196	GLY	C-N	-8.01	1.21	1.33
2	F	13[A]	HIS	CD2-NE2	-7.77	1.29	1.37
2	F	13[B]	HIS	CD2-NE2	-7.77	1.29	1.37
1	D	199	HIS	CG-ND1	-7.46	1.30	1.38
1	D	91	HIS	CD2-NE2	-6.58	1.30	1.37
1	D	44	GLY	N-CA	6.49	1.52	1.45
1	D	147	LYS	CA-CB	6.30	1.57	1.53
1	D	27	CYS	CA-CB	5.86	1.59	1.53
1	D	114	PHE	CA-CB	-5.67	1.43	1.53
1	D	199	HIS	CD2-NE2	-5.57	1.31	1.37
1	D	91	HIS	CG-ND1	-5.47	1.32	1.38
1	D	83	HIS	CD2-NE2	-5.46	1.31	1.37
2	F	13[A]	HIS	CG-ND1	-5.46	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	13[B]	HIS	CG-ND1	-5.46	1.32	1.38
1	D	29	TRP	N-CA	5.40	1.52	1.46
1	D	19	GLY	N-CA	5.39	1.50	1.45
1	D	182	CYS	N-CA	5.21	1.52	1.46
1	D	57	HIS	CD2-NE2	-5.20	1.32	1.37
1	D	245	ARG	CA-CB	5.15	1.62	1.53
1	D	127	TRP	NE1-CE2	-5.15	1.31	1.37
1	D	237	TRP	CG-CD2	-5.15	1.34	1.43
1	D	78	GLY	N-CA	5.04	1.50	1.45

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	78	GLY	N-CA-C	-10.45	100.78	111.85
1	D	76	GLU	OE1-CD-OE2	9.01	144.52	122.90
1	D	199	HIS	CA-CB-CG	-8.75	105.05	113.80
1	D	26	GLU	N-CA-C	8.74	121.60	111.11
1	D	72	ASN	CA-CB-CG	-8.47	104.13	112.60
1	D	199	HIS	N-CA-C	-8.28	93.28	108.02
1	D	57	HIS	CA-CB-CG	7.94	121.74	113.80
1	D	39	GLU	N-CA-C	-7.81	96.66	109.40
1	D	19	GLY	N-CA-C	-7.79	98.39	110.77
1	D	181	PHE	CA-CB-CG	7.76	121.56	113.80
1	D	237	TRP	N-CA-C	-7.68	102.60	110.97
1	D	212	ILE	N-CA-C	-7.60	97.18	108.12
1	D	222	ARG	N-CA-C	-7.56	96.90	109.07
2	F	14	GLU	N-CA-C	-7.55	96.59	108.90
1	D	248	PRO	N-CA-C	7.52	127.95	112.47
1	D	107	ARG	N-CA-C	-7.46	96.73	108.90
1	D	203	PHE	N-CA-C	-7.42	96.85	109.24
1	D	218	GLY	N-CA-C	-7.37	104.03	112.29
1	D	135	THR	N-CA-CB	-7.30	100.03	111.56
1	D	234	PHE	CA-CB-CG	-7.27	106.53	113.80
1	D	100	ASP	N-CA-C	-7.14	98.96	110.32
1	D	121	ALA	N-CA-C	-7.09	98.67	109.95
1	D	190	ALA	N-CA-C	-7.05	99.06	110.20
1	D	180	MET	CA-C-O	-6.99	113.26	121.44
1	D	136	GLY	N-CA-C	-6.95	100.99	111.14
1	D	203	PHE	CA-CB-CG	-6.80	107.00	113.80
1	D	176	ILE	N-CA-C	-6.59	96.17	107.24
2	F	25	ARG	N-CA-C	-6.53	99.88	110.20
2	F	29	LEU	N-CA-C	-6.53	99.89	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	117	ASN	CA-CB-CG	-6.48	106.12	112.60
1	D	215	TRP	NE1-CE2-CZ2	6.47	139.80	130.10
1	D	174	PHE	CA-CB-CG	-6.38	107.42	113.80
1	D	237	TRP	CG-CD1-NE1	-6.34	101.96	110.20
1	D	76	GLU	N-CA-C	-6.33	98.05	108.76
1	D	133	GLN	N-CA-C	-6.33	101.61	110.35
1	D	99	TYR	N-CA-C	-6.24	103.31	111.74
2	F	17	ASN	OD1-CG-ND2	-6.23	116.37	122.60
2	F	39	THR	N-CA-C	-6.22	106.32	114.04
1	D	168	CYS	N-CA-C	-6.10	103.37	111.24
2	F	11	PHE	CA-C-O	-6.10	114.33	121.16
1	D	76	GLU	CG-CD-OE1	-6.09	104.40	118.40
1	D	237	TRP	NE1-CE2-CZ2	6.04	139.17	130.10
1	D	229	THR	N-CA-C	-6.02	101.58	110.48
2	F	10	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	D	127	TRP	CG-CD1-NE1	-5.87	102.56	110.20
1	D	200	VAL	N-CA-CB	-5.87	101.18	111.39
1	D	29	TRP	NE1-CE2-CZ2	5.76	138.74	130.10
1	D	123	LEU	N-CA-C	-5.72	101.33	109.62
1	D	38	ASN	OD1-CG-ND2	-5.71	116.89	122.60
1	D	175	ILE	O-C-N	5.68	127.65	122.65
1	D	201	THR	CA-CB-OG1	-5.68	101.08	109.60
1	D	117	ASN	OD1-CG-ND2	-5.59	117.00	122.60
1	D	51	TYR	N-CA-C	5.58	118.83	109.95
1	D	179	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	D	92	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	D	215	TRP	CG-CD1-NE1	-5.45	103.12	110.20
1	D	225	TYR	N-CA-C	-5.41	101.90	109.69
1	D	130	SER	N-CA-C	5.40	118.08	111.82
2	F	4	ASP	N-CA-C	-5.39	102.35	110.06
1	D	215	TRP	NE1-CE2-CD2	-5.35	100.45	107.40
1	D	82	VAL	N-CA-C	-5.34	100.50	108.46
1	D	113	THR	N-CA-C	-5.34	97.81	107.75
1	D	83	HIS	CA-CB-CG	-5.32	108.48	113.80
1	D	177	THR	N-CA-CB	-5.30	101.98	110.51
1	D	90	LYS	N-CA-C	-5.29	100.78	109.40
1	D	208	PHE	CA-C-O	-5.28	115.14	121.11
1	D	86	GLU	N-CA-C	-5.27	105.98	112.72
1	D	35	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	D	53	LEU	N-CA-C	-5.26	100.83	109.40
1	D	39	GLU	CA-C-N	-5.23	116.73	122.38
1	D	39	GLU	C-N-CA	-5.23	116.73	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	11	PHE	O-C-N	5.22	129.26	122.89
1	D	215	TRP	CD1-NE1-CE2	5.20	118.27	108.90
1	D	241	SER	CA-CB-OG	-5.20	100.69	111.10
2	F	19	VAL	N-CA-C	-5.20	100.26	107.80
2	F	16	GLN	N-CA-CB	-5.19	103.82	111.71
1	D	185(A)	ASP	CA-CB-CG	-5.17	107.44	112.60
1	D	213	VAL	N-CA-C	-5.17	102.40	109.37
1	D	131	THR	N-CA-C	5.16	119.54	112.68
1	D	132	THR	N-CA-C	-5.16	106.30	112.59
1	D	83	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
1	D	127	TRP	NE1-CE2-CZ2	5.09	137.74	130.10
1	D	20	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	D	131	THR	CA-CB-OG1	-5.04	102.04	109.60
2	F	6	GLY	CA-C-N	5.04	131.16	121.54
2	F	6	GLY	C-N-CA	5.04	131.16	121.54
2	F	17	ASN	CB-CG-ND2	5.02	123.93	116.40

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
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 ⓘ

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	53	4
2	F	393	355	355	22	12
3	D	354	708	0	12	45
3	F	100	200	0	14	21
All	All	2754	3142	2229	73	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 16.

All (73) 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:D:90:LYS:NZ	3:D:300:HOH:O	1.57	1.27
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
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
2:F:7:ASP:CG	3:F:71:HOH:O	2.18	0.86
1:D:92:ASN:O	3:D:601:HOH:O	1.98	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:131(B):MET:HE2	1.93	0.50
1:D:131(B):MET:CE	1:D:162:TYR:CE1	2.95	0.50
1:D:240:ARG:HE	1:D:249:LYS:HZ1	1.60	0.50
1:D:131(B):MET:HE2	1:D:162:TYR:CZ	2.47	0.49
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
1:D:203:PHE:O	1:D:204:LYS:C	2.57	0.47
2:F:1:CYS:O	2:F:2:SER:C	2.58	0.47
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:92:ASN:C	3:D:601:HOH:O	2.55	0.45
1:D:27:CYS:SG	1:D:157:MET:HE3	2.58	0.44
1:D:45:THR:HG21	1:D:209:VAL:HG11	1.98	0.44
2:F:2:SER:O	2:F:3:LEU:C	2.61	0.43
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
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
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:124(A):GLU:O	1:D:125:ARG:C	2.63	0.41
1:D:122:CYS:SG	2:F:44:CYS:O	2.78	0.41
1:D:135:THR:HA	1:D:161:PRO:HA	2.02	0.41
1:D:18:GLY:HA3	1:D:146:GLU:CD	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131(B):MET:HE2	1:D:162:TYR:CE1	2.55	0.41
2:F:5:ASN:C	2:F:7:ASP:H	2.29	0.41
1:D:72:ASN:O	1:D:73:THR:C	2.64	0.41
1:D:131(B):MET:HE1	1:D:162:TYR:CE1	2.54	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 distance (Å)	Clash 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	1	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 ⓘ

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%)	179 (87%)	26 (13%)	4	1
2	F	45/82 (55%)	40 (89%)	5 (11%)	6	1
All	All	250/299 (84%)	219 (88%)	31 (12%)	5	1

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	23	LYS
1	D	37	GLU
1	D	63	ARG
1	D	73	THR
1	D	74	GLU
1	D	87	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	88	VAL
1	D	92	ASN
1	D	97	GLU
1	D	98	THR
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	173	SER
1	D	195[A]	SER
1	D	195[B]	SER
1	D	210	THR
1	D	227	ILE
1	D	232	THR
1	D	235	LEU
1	D	245	ARG
1	D	247	LEU
1	D	249	LYS
2	F	2	SER
2	F	22	SER
2	F	28	THR
2	F	39	THR
2	F	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	30	GLN
1	D	38	ASN
1	D	92	ASN
1	D	145	HIS

5.3.3 RNA ⓘ

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 oligosaccharides 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](#)

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	D	239/255 (93%)	-0.91	4 (1%)	69 76	4, 28, 58, 79	30 (12%)
2	F	52/96 (54%)	-0.88	1 (1%)	66 74	5, 24, 62, 84	11 (21%)
All	All	291/351 (82%)	-0.91	5 (1%)	69 76	4, 28, 59, 84	41 (14%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	148	GLY	3.8
1	D	146	GLU	3.3
2	F	51	ARG	2.7
1	D	151	GLN	2.2
1	D	72	ASN	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.