



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 AM UTC

PDB ID : 2UY1 / pdb_00002uy1
Title : CRYSTAL STRUCTURE OF CSTF-77
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Deposited on : 2007-04-02
Resolution : 2.00 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

<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

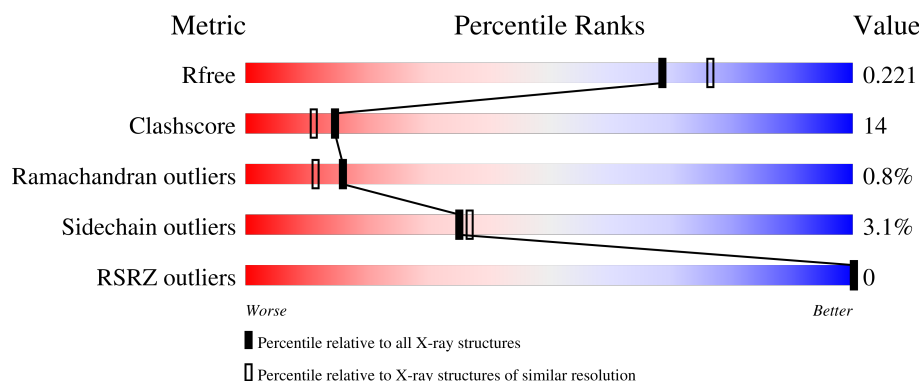
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 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	A	493	 62% 23% • • 11%
2	B	493	 53% 22% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7223 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 CLEAVAGE STIMULATION FACTOR 77.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	2	0
			3668	2374	601	672	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLU	LEU	conflict	UNP Q8SWC5

- Molecule 2 is a protein called CLEAVAGE STIMULATION FACTOR 77.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	384	Total	C	N	O	S	0	1	0
			3235	2112	530	574	19			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	TRP	LYS	conflict	UNP Q8SWC5
B	68	PHE	TYR	conflict	UNP Q8SWC5
B	88	PHE	TYR	conflict	UNP Q8SWC5
B	152	LEU	ILE	conflict	UNP Q8SWC5
B	210	PHE	TYR	conflict	UNP Q8SWC5

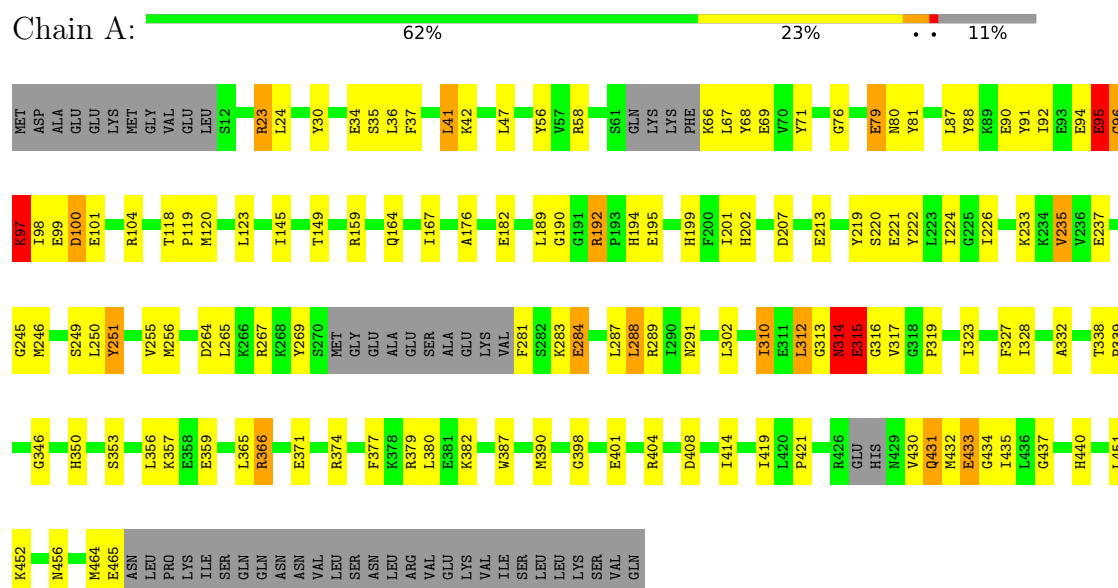
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	99	Total	O	0	0
			99	99		

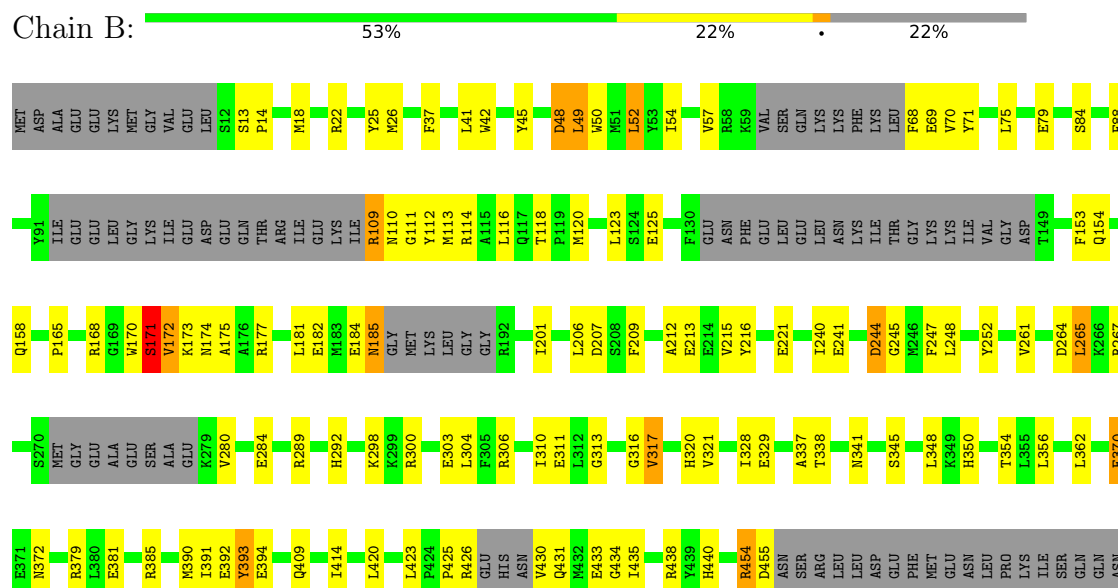
3 Residue-property plots

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: CLEAVAGE STIMULATION FACTOR 77



• Molecule 2: CLEAVAGE STIMULATION FACTOR 77



ASN
VAL
LEU
SER
ASN
LEU
ARG
VAL
GLU
LYS
VAL
ILE
SER
LEU
LYS
SER
VAL
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.44Å 148.28Å 91.44Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	91.29 – 2.00 91.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (91.29-2.00) 99.3 (91.29-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.280 0.227 , 0.221	Depositor DCC
R_{free} test set	3954 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7223	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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	A	1.41	19/3757 (0.5%)	1.28	25/5041 (0.5%)
2	B	1.19	13/3319 (0.4%)	1.23	22/4455 (0.5%)
All	All	1.31	32/7076 (0.5%)	1.26	47/9496 (0.5%)

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	A	0	8
2	B	0	4
All	All	0	12

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	TYR	C-N	-22.17	1.02	1.33
1	A	95[A]	GLU	CA-C	11.94	1.68	1.52
1	A	95[B]	GLU	CA-C	11.94	1.68	1.52
1	A	235	VAL	CA-CB	8.40	1.63	1.54
2	B	372	ASN	CG-OD1	7.08	1.36	1.23
1	A	456	ASN	CG-OD1	6.86	1.36	1.23
2	B	185	ASN	CG-OD1	6.25	1.35	1.23
1	A	332	ALA	CA-CB	6.11	1.63	1.53
2	B	391	ILE	CA-CB	6.06	1.62	1.54
1	A	255	VAL	CA-CB	6.04	1.62	1.54
2	B	48	ASP	C-O	-5.82	1.16	1.23
2	B	393	TYR	N-CA	5.76	1.52	1.46
2	B	292	HIS	ND1-CE1	5.76	1.38	1.32
2	B	350	HIS	ND1-CE1	5.64	1.38	1.32
1	A	359	GLU	C-O	-5.53	1.17	1.24
1	A	202	HIS	CD2-NE2	-5.49	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	ILE	CA-CB	5.37	1.61	1.54
2	B	50	TRP	C-O	-5.36	1.18	1.24
1	A	95[A]	GLU	N-CA	-5.35	1.39	1.46
1	A	95[B]	GLU	N-CA	-5.35	1.39	1.46
1	A	310	ILE	CA-CB	5.35	1.60	1.54
1	A	350	HIS	ND1-CE1	5.34	1.37	1.32
1	A	213	GLU	N-CA	5.31	1.53	1.46
2	B	321	VAL	CA-CB	5.31	1.61	1.54
1	A	323	ILE	CA-CB	5.30	1.60	1.54
2	B	431	GLN	CD-OE1	5.30	1.33	1.23
1	A	97	LYS	C-N	5.18	1.40	1.33
2	B	320	HIS	ND1-CE1	5.17	1.37	1.32
1	A	176	ALA	N-CA	5.16	1.52	1.46
1	A	431	GLN	CD-OE1	5.12	1.33	1.23
2	B	174	ASN	C-O	-5.11	1.17	1.24
2	B	303	GLU	C-O	-5.04	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95[A]	GLU	CA-C-O	-10.53	105.46	120.51
1	A	95[B]	GLU	CA-C-O	-10.53	105.46	120.51
2	B	454	ARG	N-CA-C	9.11	121.38	110.44
1	A	315	GLU	N-CA-C	7.59	122.20	112.34
1	A	251	TYR	CA-C-N	7.49	133.22	120.71
1	A	251	TYR	C-N-CA	7.49	133.22	120.71
1	A	312	LEU	N-CA-C	7.47	120.87	111.69
2	B	370	GLU	N-CA-C	7.13	118.70	111.07
2	B	320	HIS	CB-CG-CD2	-6.85	122.29	131.20
2	B	440	HIS	CB-CG-CD2	-6.81	122.34	131.20
1	A	302	LEU	N-CA-C	6.69	119.43	111.33
1	A	94	GLU	N-CA-C	6.63	118.30	111.14
2	B	350	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	A	350	HIS	CB-CG-CD2	-6.52	122.72	131.20
2	B	245	GLY	N-CA-C	6.44	120.88	112.25
1	A	251	TYR	O-C-N	-6.38	114.88	122.15
2	B	356	LEU	CA-CB-CG	6.24	138.13	116.30
1	A	328	ILE	N-CA-C	-6.20	104.46	110.72
1	A	202	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	291	ASN	N-CA-C	6.15	118.96	111.82
2	B	292	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	A	327	PHE	N-CA-C	6.03	117.52	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	ASP	N-CA-C	-5.95	101.74	110.42
2	B	320	HIS	CB-CG-ND1	5.83	131.45	122.70
2	B	171	SER	CA-C-N	5.78	129.76	121.55
2	B	171	SER	C-N-CA	5.78	129.76	121.55
1	A	421	PRO	CA-C-N	5.72	125.67	119.78
1	A	421	PRO	C-N-CA	5.72	125.67	119.78
2	B	409	GLN	N-CA-C	5.61	117.07	111.07
2	B	440	HIS	CB-CG-ND1	5.57	131.06	122.70
2	B	350	HIS	CB-CG-ND1	5.51	130.97	122.70
1	A	202	HIS	CB-CG-ND1	5.51	130.96	122.70
2	B	329	GLU	N-CA-C	-5.50	105.37	111.36
1	A	350	HIS	CB-CG-ND1	5.44	130.86	122.70
1	A	87	LEU	N-CA-C	5.41	116.86	111.07
2	B	328	ILE	CB-CA-C	-5.37	104.90	112.14
1	A	41	LEU	N-CA-C	5.35	116.81	110.97
1	A	88	TYR	N-CA-C	5.32	117.08	111.28
2	B	394	GLU	N-CA-C	5.31	117.48	111.11
2	B	292	HIS	CB-CG-ND1	5.12	130.38	122.70
1	A	190	GLY	N-CA-C	-5.12	105.39	112.25
1	A	164	GLN	CA-C-N	-5.09	114.42	119.56
1	A	164	GLN	C-N-CA	-5.09	114.42	119.56
2	B	393	TYR	N-CA-C	5.07	117.21	111.02
1	A	440	HIS	N-CA-C	5.06	117.45	111.33
2	B	244	ASP	N-CA-C	5.04	119.91	113.55
2	B	338	THR	O-C-N	5.03	124.35	120.38

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	LEU	Peptide
1	A	314	ASN	Peptide
1	A	95[A]	GLU	Peptide,Mainchain
1	A	95[B]	GLU	Peptide,Mainchain
1	A	96	GLY	Peptide
1	A	97	LYS	Peptide
2	B	109	ARG	Peptide
2	B	114	ARG	Peptide
2	B	170	TRP	Peptide
2	B	171	SER	Peptide

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	3668	0	3621	91	0
2	B	3235	0	3180	107	0
3	A	221	0	0	12	0
3	B	99	0	0	11	0
All	All	7223	0	6801	190	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 14.

All (190) 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:B:109:ARG:HA	2:B:111:GLY:N	1.37	1.37
2:B:109:ARG:CA	2:B:111:GLY:H	1.37	1.35
2:B:45:TYR:HB2	2:B:207:ASP:OD2	1.42	1.19
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.09	1.12
2:B:171:SER:HB3	2:B:175:ALA:H	1.08	1.09
2:B:171:SER:HB2	2:B:172:VAL:C	1.79	1.08
1:A:414:ILE:HG12	2:B:430:VAL:HG22	1.43	1.00
2:B:171:SER:CB	2:B:175:ALA:H	1.75	1.00
1:A:233:LYS:HB2	1:A:256:MET:HE2	1.47	0.96
2:B:171:SER:HB3	2:B:175:ALA:N	1.83	0.94
2:B:18:MET:HE2	2:B:48:ASP:HB3	1.51	0.92
2:B:171:SER:HA	3:B:2016:HOH:O	1.69	0.92
1:A:314:ASN:HA	1:A:316:GLY:N	1.88	0.88
2:B:212:ALA:O	2:B:215:VAL:HG22	1.73	0.87
2:B:45:TYR:CB	2:B:207:ASP:OD2	2.23	0.87
2:B:18:MET:HE1	2:B:52:LEU:HD12	1.54	0.86
2:B:165:PRO:O	2:B:168:ARG:O	1.96	0.84
2:B:116:LEU:HD22	2:B:153:PHE:HB2	1.61	0.79
1:A:58:ARG:HG2	1:A:67:LEU:HD11	1.63	0.79
2:B:48:ASP:O	2:B:49:LEU:HB3	1.83	0.78
2:B:48:ASP:O	2:B:49:LEU:CB	2.28	0.78
1:A:315:GLU:O	1:A:315:GLU:HG3	1.85	0.76
1:A:310:ILE:O	1:A:313:GLY:HA3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASN:HA	1:A:316:GLY:H	1.51	0.75
1:A:42:LYS:HG2	3:A:2010:HOH:O	1.87	0.74
2:B:171:SER:HB2	2:B:173:LYS:N	2.02	0.74
2:B:425:PRO:O	2:B:426:ARG:HB2	1.88	0.74
1:A:192:ARG:HG2	1:A:192:ARG:NH1	1.87	0.74
2:B:109:ARG:HA	2:B:111:GLY:CA	2.17	0.74
1:A:246:MET:O	1:A:250:LEU:HG	1.88	0.73
2:B:25:TYR:HD2	2:B:26:MET:HE3	1.54	0.72
2:B:109:ARG:HA	2:B:111:GLY:H	0.58	0.72
1:A:99:GLU:O	1:A:100:ASP:CB	2.38	0.71
1:A:433:GLU:HB3	2:B:414:ILE:HG21	1.73	0.71
1:A:233:LYS:O	1:A:237:GLU:HG3	1.90	0.70
1:A:96:GLY:HA3	1:A:97:LYS:CB	2.22	0.69
2:B:18:MET:CE	2:B:48:ASP:HB3	2.22	0.68
2:B:289:ARG:HH11	2:B:317:VAL:HG12	1.57	0.67
2:B:171:SER:OG	2:B:172:VAL:HA	1.96	0.66
1:A:182:GLU:HG3	1:A:201:ILE:CD1	2.25	0.66
2:B:171:SER:CB	2:B:172:VAL:CA	2.74	0.66
2:B:289:ARG:NH1	2:B:317:VAL:HG12	2.10	0.65
2:B:171:SER:CB	2:B:172:VAL:C	2.66	0.64
1:A:366:ARG:HD2	3:A:2146:HOH:O	1.96	0.64
2:B:171:SER:HB2	2:B:172:VAL:CA	2.27	0.64
1:A:377:PHE:CG	1:A:390:MET:HE2	2.33	0.63
1:A:374:ARG:HA	1:A:390:MET:HE1	1.80	0.63
2:B:241:GLU:HG2	3:B:2026:HOH:O	1.97	0.62
2:B:379:ARG:HD3	3:B:2059:HOH:O	1.99	0.62
1:A:264:ASP:OD1	1:A:267:ARG:NH2	2.33	0.62
2:B:25:TYR:CD2	2:B:26:MET:HE3	2.35	0.62
2:B:18:MET:HE1	2:B:52:LEU:CD1	2.29	0.61
1:A:145:ILE:O	1:A:149:THR:HG23	2.00	0.61
2:B:109:ARG:CA	2:B:111:GLY:N	2.23	0.60
2:B:182:GLU:HG3	2:B:201:ILE:CD1	2.31	0.59
2:B:125:GLU:N	2:B:125:GLU:OE1	2.37	0.58
2:B:109:ARG:C	2:B:111:GLY:H	2.01	0.58
1:A:353:SER:O	1:A:357:LYS:HG3	2.03	0.58
1:A:47:LEU:HD22	1:A:81:TYR:HE2	1.68	0.58
1:A:99:GLU:O	1:A:100:ASP:HB2	2.04	0.57
2:B:26:MET:HA	2:B:26:MET:HE2	1.86	0.57
1:A:404:ARG:NH2	2:B:221:GLU:OE1	2.36	0.57
1:A:408:ASP:OD1	2:B:438:ARG:NH1	2.30	0.56
1:A:80:ASN:HA	1:A:118:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:C	1:A:98:ILE:H	2.14	0.56
2:B:158:GLN:HG2	3:B:2013:HOH:O	2.07	0.55
2:B:88:PHE:CD1	2:B:120:MET:HE1	2.42	0.54
1:A:432:MET:HB2	1:A:437:GLY:HA2	1.89	0.54
1:A:30:TYR:O	1:A:34:GLU:HG3	2.08	0.54
2:B:215:VAL:HG23	2:B:216:TYR:CD2	2.43	0.54
2:B:45:TYR:N	2:B:207:ASP:OD2	2.41	0.53
1:A:189:LEU:HD23	1:A:194:HIS:HA	1.89	0.53
1:A:76:GLY:O	1:A:79:GLU:HG2	2.08	0.53
2:B:311:GLU:C	2:B:313:GLY:H	2.17	0.53
2:B:311:GLU:HG3	3:B:2040:HOH:O	2.08	0.53
1:A:452:LYS:HE2	3:A:2194:HOH:O	2.08	0.52
2:B:70:VAL:HG12	2:B:70:VAL:O	2.09	0.52
1:A:281:PHE:HA	1:A:284:GLU:OE2	2.09	0.52
2:B:116:LEU:HA	2:B:123:LEU:HD11	1.91	0.52
2:B:370:GLU:OE1	2:B:393:TYR:OH	2.17	0.52
1:A:68:TYR:HB2	1:A:95[B]:GLU:OE2	2.09	0.52
2:B:18:MET:CE	2:B:52:LEU:HD12	2.34	0.52
2:B:171:SER:OG	2:B:172:VAL:CA	2.57	0.52
3:A:2189:HOH:O	2:B:433:GLU:HG3	2.09	0.51
1:A:219:TYR:HB3	1:A:235:VAL:HG11	1.91	0.51
2:B:68:PHE:HA	2:B:71:TYR:HD2	1.75	0.51
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.00	0.51
2:B:392:GLU:OE2	3:B:2068:HOH:O	2.19	0.51
2:B:45:TYR:CA	2:B:207:ASP:OD2	2.59	0.51
2:B:54:ILE:HA	2:B:57:VAL:HG12	1.91	0.51
2:B:79:GLU:O	2:B:118:THR:HG21	2.10	0.51
1:A:357:LYS:HB3	1:A:380:LEU:HD13	1.92	0.50
2:B:18:MET:CE	2:B:52:LEU:CD1	2.90	0.50
1:A:404:ARG:HH22	2:B:221:GLU:CD	2.19	0.50
2:B:18:MET:HE2	2:B:48:ASP:CB	2.34	0.50
2:B:154:GLN:O	2:B:158:GLN:HG3	2.11	0.50
2:B:213:GLU:HB2	2:B:248:LEU:HG	1.93	0.50
2:B:252:TYR:HD2	2:B:261:VAL:HG11	1.76	0.50
2:B:454:ARG:O	2:B:455:ASP:OD1	2.30	0.49
1:A:182:GLU:HG3	1:A:201:ILE:HD11	1.94	0.49
2:B:306:ARG:O	2:B:310:ILE:HG13	2.12	0.49
2:B:454:ARG:O	2:B:455:ASP:CG	2.56	0.49
1:A:96:GLY:HA3	1:A:97:LYS:HB3	1.94	0.49
2:B:264:ASP:OD1	2:B:267:ARG:NH2	2.45	0.49
1:A:34:GLU:OE2	1:A:56:TYR:OH	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ARG:HD2	2:B:112:TYR:CD1	2.48	0.48
1:A:101:GLU:HG3	1:A:104:ARG:NH2	2.27	0.48
1:A:96:GLY:HA3	1:A:97:LYS:HB2	1.93	0.48
2:B:171:SER:CA	3:B:2016:HOH:O	2.42	0.48
1:A:99:GLU:O	1:A:100:ASP:HB3	2.12	0.47
2:B:49:LEU:CD2	3:B:2001:HOH:O	2.63	0.47
1:A:36:LEU:C	1:A:36:LEU:HD23	2.40	0.47
2:B:284:GLU:H	2:B:284:GLU:HG2	1.33	0.47
1:A:118:THR:HB	1:A:120:MET:CE	2.44	0.47
1:A:246:MET:O	1:A:246:MET:HG3	2.14	0.47
1:A:464:MET:O	1:A:465:GLU:HB2	2.12	0.47
2:B:390:MET:HE3	2:B:390:MET:HA	1.97	0.47
2:B:433:GLU:CG	2:B:434:GLY:N	2.79	0.47
1:A:119:PRO:HD3	1:A:159:ARG:NH2	2.30	0.46
1:A:379:ARG:NH2	3:A:2169:HOH:O	2.37	0.46
2:B:433:GLU:HG2	2:B:434:GLY:N	2.31	0.46
2:B:354:THR:HG22	2:B:423:LEU:HD21	1.98	0.46
2:B:381:GLU:HG3	3:B:2060:HOH:O	2.14	0.46
1:A:371:GLU:HG3	3:A:2166:HOH:O	2.15	0.46
1:A:195[A]:GLU:HG2	1:A:199:HIS:CD2	2.51	0.46
2:B:337:ALA:O	2:B:341:ASN:ND2	2.43	0.46
1:A:96:GLY:C	1:A:98:ILE:N	2.74	0.46
1:A:319:PRO:HB3	1:A:356:LEU:HD22	1.97	0.46
2:B:265:LEU:HD12	2:B:265:LEU:HA	1.77	0.46
1:A:289:ARG:HD3	1:A:317:VAL:HG12	1.98	0.45
1:A:401:GLU:HG2	3:A:2185:HOH:O	2.16	0.45
2:B:109:ARG:C	2:B:111:GLY:N	2.65	0.45
2:B:109:ARG:HD2	2:B:112:TYR:HD1	1.81	0.45
2:B:48:ASP:O	2:B:49:LEU:HB2	2.14	0.45
1:A:377:PHE:CB	1:A:390:MET:HE2	2.46	0.45
2:B:171:SER:C	3:B:2016:HOH:O	2.59	0.45
2:B:430:VAL:HG12	2:B:430:VAL:O	2.16	0.45
2:B:209:PHE:HB2	2:B:215:VAL:HG11	1.99	0.45
1:A:80:ASN:HB2	3:A:2024:HOH:O	2.15	0.44
2:B:22:ARG:HG3	2:B:22:ARG:HH11	1.82	0.44
1:A:23:ARG:HD3	3:A:2006:HOH:O	2.17	0.44
1:A:249:SER:HB3	1:A:265:LEU:HD11	1.99	0.44
1:A:419:ILE:HG13	2:B:430:VAL:HG21	1.99	0.44
2:B:300:ARG:HB3	2:B:304:LEU:HD12	1.99	0.44
2:B:184:GLU:HG3	2:B:185:ASN:H	1.82	0.44
2:B:435:ILE:HD12	2:B:438:ARG:HD2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLN:C	1:A:432:MET:HE2	2.43	0.43
1:A:71:TYR:OH	1:A:90:GLU:OE1	2.27	0.43
2:B:240:ILE:O	3:B:2027:HOH:O	2.21	0.43
1:A:221:GLU:OE2	1:A:251:TYR:OH	2.32	0.43
2:B:213:GLU:CD	2:B:247:PHE:HB3	2.44	0.43
1:A:91:TYR:CE1	1:A:95[B]:GLU:OE2	2.72	0.43
2:B:68:PHE:C	2:B:70:VAL:H	2.25	0.43
2:B:381:GLU:HB2	2:B:420:LEU:HD11	1.99	0.43
2:B:345:SER:HA	2:B:348:LEU:HD12	2.01	0.43
2:B:37:PHE:HE1	2:B:49:LEU:HD12	1.83	0.43
2:B:75:LEU:O	2:B:79:GLU:HB3	2.19	0.43
1:A:338:THR:HB	1:A:339:PRO:CD	2.49	0.42
1:A:346:GLY:C	1:A:356:LEU:HD21	2.45	0.42
1:A:42:LYS:HG2	1:A:42:LYS:H	1.51	0.42
1:A:220:SER:O	1:A:224:ILE:HG13	2.19	0.42
1:A:287:LEU:HG	1:A:451:LEU:HB3	1.99	0.42
3:A:2178:HOH:O	2:B:298:LYS:HE2	2.19	0.42
1:A:419:ILE:HG13	2:B:430:VAL:CG2	2.50	0.42
1:A:267:ARG:C	1:A:269:TYR:H	2.28	0.42
2:B:84:SER:OG	2:B:120:MET:HE2	2.20	0.42
2:B:173:LYS:NZ	2:B:177:ARG:NH2	2.68	0.41
1:A:37:PHE:O	1:A:41:LEU:HB2	2.20	0.41
1:A:66:LYS:O	1:A:69:GLU:HB2	2.20	0.41
1:A:167:ILE:HD12	1:A:167:ILE:HG23	1.88	0.41
1:A:398:GLY:O	2:B:298:LYS:HE3	2.20	0.41
1:A:382:LYS:HD3	1:A:387:TRP:CE2	2.56	0.41
1:A:120:MET:HG2	1:A:123:LEU:HD13	2.02	0.41
1:A:256:MET:HA	1:A:256:MET:HE3	2.03	0.41
2:B:70:VAL:O	2:B:70:VAL:CG1	2.68	0.41
1:A:314:ASN:CA	1:A:316:GLY:H	2.25	0.41
1:A:379:ARG:HD3	3:A:2170:HOH:O	2.21	0.41
2:B:379:ARG:HE	2:B:379:ARG:HB3	1.57	0.41
1:A:92:ILE:HA	1:A:95[A]:GLU:OE1	2.21	0.41
1:A:245:GLY:HA3	3:A:2110:HOH:O	2.20	0.41
1:A:288:LEU:HD23	1:A:289:ARG:HG3	2.01	0.41
1:A:192:ARG:NH1	1:A:192:ARG:CG	2.67	0.40
1:A:222:TYR:CZ	1:A:226:ILE:HD13	2.56	0.40
1:A:284:GLU:H	1:A:284:GLU:CD	2.29	0.40
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.87	0.40
2:B:41:LEU:O	2:B:42:TRP:C	2.62	0.40
1:A:118:THR:HB	1:A:120:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:LEU:HD11	2:B:385:ARG:HD3	2.03	0.40
2:B:13:SER:O	2:B:14:PRO:C	2.64	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	432/493 (88%)	412 (95%)	17 (4%)	3 (1%)	18	14
2	B	371/493 (75%)	358 (96%)	10 (3%)	3 (1%)	16	11
All	All	803/986 (81%)	770 (96%)	27 (3%)	6 (1%)	16	14

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	314	ASN
2	B	49	LEU
2	B	110	ASN
2	B	316	GLY
1	A	434	GLY

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	395/444 (89%)	382 (97%)	13 (3%)	33	34
2	B	346/444 (78%)	336 (97%)	10 (3%)	37	40
All	All	741/888 (83%)	718 (97%)	23 (3%)	35	37

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	35	SER
1	A	79	GLU
1	A	192	ARG
1	A	207	ASP
1	A	283	LYS
1	A	284	GLU
1	A	288	LEU
1	A	315	GLU
1	A	365	LEU
1	A	366	ARG
1	A	430	VAL
1	A	433	GLU
2	B	52	LEU
2	B	69	GLU
2	B	113	MET
2	B	172	VAL
2	B	181	LEU
2	B	206	LEU
2	B	244	ASP
2	B	265	LEU
2	B	280	VAL
2	B	317	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	174	ASN
1	A	203	ASN
2	B	203	ASN
2	B	228	GLN
2	B	409	GLN

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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	251:TYR	C	252:TYR	N	1.02

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	A	438/493 (88%)	-1.48	0 100 100	11, 22, 44, 58	2 (0%)
2	B	384/493 (77%)	-1.30	0 100 100	7, 31, 52, 61	1 (0%)
All	All	822/986 (83%)	-1.40	0 100 100	7, 26, 50, 61	3 (0%)

There are no RSRZ outliers to report.

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.